

Week	Lectur Title	Contents
1	1 Introduction to the course	<ul style="list-style-type: none"> <li>- Introduction to the course, objectives, and expectations.</li> <li>- Describe "Changing hats" sessions (and lottery)</li> <li>- Describe "Hands-on" sessions</li> <li>- Describe "Invited lecture"</li> <li>- Describe Program</li> <li>- Introduction to HPC               <ul style="list-style-type: none"> <li>- Overview of high-performance computing, its evolution, and its impact on various domains.</li> <li>- Importance of HPC in scientific research, simulations, and data-intensive applications</li> </ul> </li> <li>- Introduction to Distributed AI</li> </ul>
	2 Introduction to HPC	<ul style="list-style-type: none"> <li>- Brief history of supercomputers</li> <li>- Measuring capacity: FLOPs and memory</li> <li>- Comparing resources: from your laptop to the World's TOP10 from TOP500</li> <li>- Requirements (cooling, space, etc.) and "the first" big issue: scheduling</li> </ul>
	3 Fundamentals of HPC Architecture	<ul style="list-style-type: none"> <li>- Lookback into 102.2</li> <li>- Basics of parallel processing and its role in achieving high performance.</li> <li>- Overview of supercomputers, clusters, and distributed memory systems.</li> <li>- Introduction to GPU acceleration and its applications.</li> <li>- Mention TPU briefly</li> <li>- Brief intro to DISCO (w/focus on hardware)</li> </ul>
	4 Scheduling and environment: from PC to HPC	<ul style="list-style-type: none"> <li>- Lookback into unit 202.2 (OS and concurrence)</li> <li>- OS scheduling vs. HPC scheduling</li> <li>- HPC scheduling software &amp; SLURM (Simple Linux Utility for Resource Management):               <ul style="list-style-type: none"> <li>- Define the role of job scheduling in optimizing resource utilization</li> <li>- Highlight the challenges of managing computing resources in a multi-tenant environment.</li> <li>- Introduce SLURM as a solution for efficient job scheduling.</li> </ul> </li> <li>- Preparing environments on HPC &amp; containers</li> </ul>
2	5 SLURM	<ul style="list-style-type: none"> <li>- Architecture of SLURM               <ul style="list-style-type: none"> <li>- Explain the purpose and functionality of SLURM's control daemon (slurmctld)</li> <li>- Describe the role of SLURM's job scheduler (slurmd) on compute nodes.</li> <li>- Outline the interaction between SLURM components in managing job submissions and resource allocation</li> <li>- Introduce the concept of partitions</li> </ul> </li> <li>- Deployment of SLURM               <ul style="list-style-type: none"> <li>- Discuss the SLURM configuration file (slurm.conf) and its key parameters.</li> <li>- Demonstrate how to define partitions and resources within the configuration</li> <li>- Discuss some optimization options depending on different cluster architecture use-cases</li> </ul> </li> <li>- Job submission and management:               <ul style="list-style-type: none"> <li>- Submitting jobs with sbatch and specifying job requirements</li> <li>- Introduce a typically underestimated utility: job arrays</li> <li>- Explain how to monitor job status, resource usage, and job dependencies using various SLURM commands (squeue, scontrol)</li> <li>- Interactive sessions on nodes (srun/sdev)</li> </ul> </li> <li>- Advanced SLURM &amp; best practices               <ul style="list-style-type: none"> <li>- Strategies to parallelize across nodes (multi-node job execution)</li> <li>- Extend job arrays in parallelization</li> <li>- Mention the existence of plugins and showcase some scripting extensions (e.g., launcher)</li> <li>- Optimizing job performance and minimizing queue latencies</li> <li>- Common issues and errors (e.g., execution on login node) in SLURM usage and "good citizenship" (e.g., "nice" config)</li> </ul> </li> <li>- Provide a perspective on SLURM alternatives (Torque, PBS Pro, HTCondor, SGE)</li> </ul>
	6 Hands-on: playing with DISCO	<ul style="list-style-type: none"> <li>- A practical session where prepared (and small) programs will be launched by the students, to then track the execution by the cluster.</li> <li>- SLURM tools for post-investigation of the fate of programs. Some of the examples will intendendly be created to fail (e.g., allocating excessive memory), letting the students to investigate the problem.</li> <li>- Etiquette when using multi-tenant systems such as HPCs - login nodes, data-transfer nodes and compute nodes.</li> <li>- Define the fundamental concepts of HPC and Cloud Computing, highlighting differential points.</li> <li>- Highlight the primary differences in architecture, resource provisioning, and usage models.</li> <li>- Infrastructure Ownership               <ul style="list-style-type: none"> <li>- Discuss how HPC involves dedicated, on-premises infrastructure owned by an organization.</li> <li>- Contrast this with Cloud Computing, where infrastructure is typically owned and managed by a third-party cloud service provider.</li> </ul> </li> <li>- Resource Provisioning               <ul style="list-style-type: none"> <li>- Explain the on-demand nature of resource provisioning in Cloud Computing, allowing for flexibility and scalability.</li> <li>- Describe the static allocation of resources in HPC, where users typically have dedicated access to specific hardware.</li> </ul> </li> <li>- Security               <ul style="list-style-type: none"> <li>- Discuss security considerations in HPC, where isolated, tightly controlled environments are preferred for sensitive research and data.</li> <li>- Highlight traditional HPC practices that prioritize physical and network security within controlled environments.</li> <li>- Address security considerations in Cloud Computing, emphasizing shared infrastructure and virtualization challenges.</li> <li>- Discuss the role of cloud providers in ensuring security and the importance of robust access controls.</li> </ul> </li> <li>- Describe scenarios where each option is most efficient / useful               <ul style="list-style-type: none"> <li>- Identify scenarios where HPC is most efficient, such as complex scientific simulations, numerical modeling, and large-scale data processing.</li> <li>- Discuss the advantages of specialized hardware for compute-intensive tasks.</li> <li>- Highlight scenarios where Cloud Computing excels, including variable workloads, rapid scalability, and global accessibility.</li> <li>- Discuss the advantages of outsourcing infrastructure for cost savings and flexibility.</li> </ul> </li> </ul>
	7 HPC vs Cloud	<ul style="list-style-type: none"> <li>- Highlighting the cost, performance, and scalability implications of choosing between HPC and cloud solutions.               <ul style="list-style-type: none"> <li>- Break down the cost implications of HPC, including initial infrastructure investment and ongoing maintenance.</li> <li>- Contrast this with the pay-as-you-go model of Cloud Computing, where costs are tied to actual resource usage.</li> <li>- Discuss the performance benefits of HPC, where specialized hardware can deliver high throughput and low latency.</li> <li>- Acknowledge the performance trade-offs in Cloud Computing, where shared resources may lead to variability in performance.</li> <li>- Explore scalability considerations in both HPC and Cloud Computing.</li> <li>- Discuss how HPC scales vertically with powerful hardware, while Cloud Computing scales horizontally by adding more virtual instances.</li> </ul> </li> <li>- Deploying environments: Cloud vs. HPC               <ul style="list-style-type: none"> <li>- Detail the process of deploying environments in HPC, emphasizing custom configurations and direct hardware access.</li> <li>- Discuss how HPC environments are tailored for specific applications and workloads.</li> <li>- Outline the ease of environment deployment in Cloud Computing using virtual machines or containers.</li> <li>- Introduce containerization technologies like Docker and Kubernetes that facilitate consistent environment deployment across clouds.</li> <li>- Discuss the security challenges associated with containerization, particularly in multi-tenant environments.</li> <li>- Address concerns related to container isolation, shared kernel vulnerabilities, and container escape.</li> <li>- Introduce security-focused containerization solutions in HPC, such as Singularity (now known as Apptainer).</li> <li>- Discuss why HPC traditionally resisted Docker due to security concerns and how Singularity addresses these challenges.</li> </ul> </li> </ul>

Week	Lectur Title	Contents
3	8 Changing hats: docker / containers basics	<ul style="list-style-type: none"> <li>- Student 1: Introduction to Docker <ul style="list-style-type: none"> <li>- Introduction <ul style="list-style-type: none"> <li>- Briefly explain the concept of containerization and its significance in modern software development.</li> <li>- Introduce Docker as a popular containerization platform.</li> </ul> </li> <li>- Docker Installation Steps <ul style="list-style-type: none"> <li>- Provide step-by-step instructions for installing Docker on different operating systems (Windows, macOS, Linux).</li> <li>- Anticipate potential installation issues on various platforms and offer troubleshooting tips.</li> </ul> </li> <li>- Checking Docker Installation <ul style="list-style-type: none"> <li>- Guide participants on how to verify a successful Docker installation.</li> <li>- Demonstrate basic Docker commands like <code>docker --version</code> and <code>docker info</code>.</li> <li>- Troubleshoot common issues such as permission errors and missing dependencies.</li> </ul> </li> <li>- Running Hello World Image <ul style="list-style-type: none"> <li>- Explain the concept of Docker images and containers.</li> <li>- Walk through the process of running the "Hello World" Docker image.</li> <li>- Address potential challenges such as image download errors or connectivity issues.</li> </ul> </li> </ul> </li> <li>- Student 2: Understanding Docker Concepts <ul style="list-style-type: none"> <li>- Introduction <ul style="list-style-type: none"> <li>- Advantages of containers.</li> <li>- Introduce the core concepts: images, containers, and how they differ from virtual machines.</li> </ul> </li> <li>- Differences Between Images and Containers <ul style="list-style-type: none"> <li>- Define Docker images and containers and explain their relationship.</li> <li>- Illustrate with examples the distinction between a static image and a running container.</li> </ul> </li> <li>- Differences with Virtual Machines <ul style="list-style-type: none"> <li>- Compare and contrast containers with virtual machines.</li> <li>- Discuss resource efficiency, startup times, and resource isolation.</li> <li>- Address common misconceptions and potential challenges in transitioning from VMs to containers.</li> </ul> </li> <li>- Layers and Image Build <ul style="list-style-type: none"> <li>- Explain the concept of Docker image layers.</li> <li>- Guide participants through a functional and easy image build using a provided Dockerfile.</li> <li>- Anticipate issues related to Dockerfile syntax errors and best practices in image creation.</li> <li>- Introduce the concept of remote image repositories like Docker Hub.</li> </ul> </li> </ul> </li> <li>- Student 3: Advanced Docker Usage <ul style="list-style-type: none"> <li>- Executing containers <ul style="list-style-type: none"> <li>- Execution permissions of the docker daemon</li> <li>- Mounting filesystems points and their permissions</li> <li>- User and group binding</li> <li>- Interactive Execution of Containers</li> </ul> </li> <li>- Container Management <ul style="list-style-type: none"> <li>- Introduce basic container management commands (<code>docker ps</code>, <code>docker stop</code>, <code>docker rm</code>).</li> <li>- Discuss the significance of container names and IDs.</li> <li>- Anticipate challenges with container management, such as conflicts with container names.</li> </ul> </li> <li>- Detaching and Reattaching Containers <ul style="list-style-type: none"> <li>- Discuss scenarios where detaching and reattaching containers are useful.</li> <li>- Demonstrate how to detach from a running container without stopping it.</li> <li>- Address potential challenges with detaching and reattaching, such as terminal disconnections.</li> </ul> </li> </ul> </li></ul>
	9 Consolidate "changing hats" session	<ul style="list-style-type: none"> <li>- Consolidate the changing hats session: <ul style="list-style-type: none"> <li>- Briefly recap the key points covered by each student in the previous Changing Hats session.</li> <li>- Discuss difficult points and bring up elements that were not covered in sufficient depth or with clarity</li> </ul> </li> </ul>
	10 Deploying Environments with Containers	<ul style="list-style-type: none"> <li>- Introduction to containerization technologies (Docker, Singularity/Apptainer) and their role in deploying environments.</li> <li>- Benefits of containerization for reproducibility, portability, and ease of deployment.</li> <li>- Security: docker/kubernetes vs singularity (apptainer)</li> </ul>
4	11 Parallel and distributed computing on HPC (1)	<ul style="list-style-type: none"> <li>- Consolidate the changing hats session</li> <li>- Introduction to containerization technologies (Docker, Singularity/Apptainer) and their role in deploying environments.</li> <li>- Benefits of containerization for reproducibility, portability, and ease of deployment.</li> <li>- Security: docker/kubernetes vs singularity (apptainer)</li> <li>- Developing/debugging with containers - example with Python</li> </ul>
	12 Parallel and distributed computing on HPC (2)	<ul style="list-style-type: none"> <li>- Lookback into unit 202.2 (OS and concurrence)</li> <li>- Shared vs. distributed memory (parallel vs distributed)</li> <li>- Architectures</li> <li>- Embarrassingly parallel solutions across nodes (continuation from Lecture 5)</li> </ul>
	13 Hands-on: peer-programming	<ul style="list-style-type: none"> <li>- Overview of parallel programming models (MPI, OpenMP, CUDA).</li> <li>- Hands-on examples and exercises to reinforce programming concepts.</li> <li>- Discussing challenges and best practices in HPC programming.</li> </ul>
4	14 Managing Containers at Scale with Kubernetes	<ul style="list-style-type: none"> <li>- Use DISCO and launch a parametric job with launcher and with job-arrays</li> <li>- Create and fine tune the SLURM configuration the sbatch file for a particular application</li> <li>- Use DISCO to benchmark I/O performance on an HPC system.</li> <li>- Deploy a sample application on both HPC and a cloud platform.</li> <li>- Create a containerized environment using Docker and Singularity.</li> <li>- Develop a parallelized algorithm using MPI</li> <li>- Implement a parallelized task using OpenMP</li> <li>- Build a Docker image to execute Jupyter notebooks with an AI environment (e.g., with PyTorch)</li> <li>- Review and troubleshoot Dockerfiles from previous sessions.</li> <li>- Overview of Kubernetes and its role in orchestrating containerized applications.</li> <li>- Discussing how Kubernetes addresses challenges in deploying and managing distributed systems.</li> <li>- Practical exercises on deploying and scaling applications with Kubernetes.</li> <li>- Monitoring and Managing Resources <ul style="list-style-type: none"> <li>- Touch on the importance of monitoring resources in a Kubernetes cluster.</li> <li>- Introduce tools and practices for managing resources effectively.</li> </ul> </li> </ul>
	15 Intro to ML through scikit-learn	<ul style="list-style-type: none"> <li>- Lookback/sync with 301 (ML briefing)</li> <li>- Introduction and general design considerations</li> <li>- Navigating the documentation</li> <li>- Core functionalities and key modules.</li> <li>- Essential utilities for data manipulation and model evaluation.</li> <li>- Supervised and unsupervised learning algorithms.</li> <li>- Model evaluation using metrics.</li> <li>- Showcasing guided exercises from the documentation</li> <li>- Student 1: Feature Engineering in scikit-learn. <ul style="list-style-type: none"> <li>- Describe feature engineering techniques available in scikit-learn.</li> <li>- Discuss the impact of feature engineering on model performance.</li> <li>- Provide practical examples and case studies showcasing effective feature engineering.</li> </ul> </li> </ul>
	16 Changing hats: scikit-learn	<ul style="list-style-type: none"> <li>- Student 2: Hyperparameter Tuning with Grid Search and Random Search. <ul style="list-style-type: none"> <li>- Dive into hyperparameter tuning using Grid Search and Random Search in scikit-learn.</li> <li>- Compare the advantages and limitations of each approach.</li> <li>- Demonstrate how to implement hyperparameter tuning on a specific machine learning model.</li> </ul> </li> <li>- Student 3: Ensemble Learning in scikit-learn. <ul style="list-style-type: none"> <li>- Introduce ensemble learning concepts and algorithms available in scikit-learn.</li> <li>- Compare and contrast different ensemble methods (e.g., RandomForest, AdaBoost).</li> <li>- Present real-world applications and use cases where ensemble learning is beneficial.</li> </ul> </li> </ul>
	17 Using scikit-learn (consolidating "changing hats")	<ul style="list-style-type: none"> <li>- Consolidate the changing hats session: <ul style="list-style-type: none"> <li>- Briefly recap the key points covered by each student in the previous Changing Hats session.</li> <li>- Discuss difficult points and bring up elements that were not covered in sufficient depth or with clarity</li> </ul> </li> <li>- Feature engineering and preprocessing <ul style="list-style-type: none"> <li>- Building data pipelines</li> <li>- Cross-validation and nested cross-validation</li> <li>- Parallelization</li> <li>- Example combining a pipeline and comparing cross-validation vs. nested cross-validation</li> </ul> </li> </ul>

Week	Lectur Title	Contents
5	18 Ensemble Learning (with scikit-learn) and Distributed ML	<ul style="list-style-type: none"> <li>- Define Ensemble Learning and its motivation.</li> <li>- Ensemble Methods: <ul style="list-style-type: none"> <li>- Bagging (Bootstrap Aggregating): Reduce variance with methods like Random Forest.</li> <li>- Boosting (AdaBoost, Gradient Boosting): Correct model errors iteratively.</li> <li>- Stacking: Combine predictions from diverse models.</li> </ul> </li> <li>- Implementation and Optimization <ul style="list-style-type: none"> <li>- Considerations for setting up ensemble models.</li> <li>- Strategies for optimizing ensemble hyperparameters.</li> <li>- Metrics and techniques for assessing ensemble performance.</li> </ul> </li> <li>- Introduce Canonical Ensemble Learning as a precedent of energy-based models introduced in lecture 49.</li> <li>- Discuss how ensemble methods can be adapted and optimized for distributed machine learning environments.</li> </ul>
	19 Hands-on: peer-programming	<ul style="list-style-type: none"> <li>- Case Studies and Examples</li> <li>- Implement a Random Forest classifier using bagging.</li> <li>- Employ AdaBoost ensemble for a classification problem.</li> <li>- Build a stacking ensemble using diverse base models</li> <li>- Extend a basic ensemble training script for distributed computing</li> <li>- Modify an ensemble approach for handling large-scale datasets</li> <li>- Develop a nested cross-validation script for hyperparameter tuning of an ensemble model</li> <li>- Implement a mechanism to dynamically adjust the size of an ensemble during training</li> <li>- Integrate feature engineering techniques into the ensemble learning pipeline. Explore how feature transformations impact the overall performance of the ensemble.</li> <li>- Scale ensemble learning for a distributed computing cluster</li> <li>- Replicate and extend a case study presented in the previous session</li> <li>- Definition and significance of data pipelines in scientific computing.</li> <li>- Overview of challenges and benefits in deploying data pipelines in HPC.</li> <li>- Lookback to scikit-learn's pipelines</li> <li>- Introduction to key concepts: <ul style="list-style-type: none"> <li>- data provenance,</li> <li>- pipeline synchronization/communication,</li> <li>- resource management and allocation,</li> <li>- job dependency matrix,</li> <li>- error handling and fault tolerance,</li> <li>- reproducibility,</li> <li>- scalability.</li> </ul> </li> <li>- Deploying data pipelines on HPC</li> <li>- Understand the overlap and collaboration between data pipelines and HPC scheduling</li> </ul>
	20 Data pipelines and HPC	
6	21 Nextflow: A Scalable and Reproducible Data Workflow Engine	<ul style="list-style-type: none"> <li>- In-depth exploration of Nextflow for building scalable and reproducible workflows.</li> <li>- Hands-on demonstration of creating a simple data pipeline with Nextflow.</li> <li>- Discussion on features, syntax, and best practices.</li> </ul>
	22 Python's Dask for Parallel Computing and Scalable Data Analytics	<ul style="list-style-type: none"> <li>- Introduction to Dask and its role in parallel computing and data analytics.</li> <li>- Hands-on exercises demonstrating parallel computing with Dask.</li> <li>- Discussion on integrating Dask with HPC environments.</li> </ul>
	23 Nipype: A Python Framework for Neuroimaging Pipelines	<ul style="list-style-type: none"> <li>- Overview of Nipype and its application in neuroimaging pipelines.</li> <li>- Practical examples of building and executing neuroimaging workflows.</li> <li>- Discussion on interfacing with existing tools and ensuring reproducibility.</li> </ul>
	24 "Changing hats" session (data pipelines)	<ul style="list-style-type: none"> <li>- Student 1: A data pipeline with Nextflow, deployed on DISCO</li> <li>- Student 2: A data pipeline with Dask, deployed on DISCO</li> <li>- Student 3: A data pipeline with Nipype, deployed on DISCO</li> </ul>
7	25 Comparative Analysis of Data Pipeline Engines	<ul style="list-style-type: none"> <li>- Consolidate the changing hats session: <ul style="list-style-type: none"> <li>- Briefly recap the key points covered by each student in the previous Changing Hats session.</li> <li>- Discuss difficult points and bring up elements that were not covered in sufficient depth or with clarity</li> </ul> </li> <li>- Comparative review of Nextflow, Dask, Nipype, and other notable engines.</li> <li>- Strengths, weaknesses, and use cases for each engine.</li> <li>- Learn how to introspect the pipeline and understand the bottlenecks of execution</li> <li>- Discussion on choosing the right engine based on specific requirements.</li> <li>- Build a basic Nextflow workflow: Create a simple Nextflow workflow with two processes.</li> <li>- Parallelize data processing with Dask: Use Dask to parallelize a data processing task.</li> <li>- Nipype for neuroimaging pipeline: Construct a Nipype pipeline for a basic neuroimaging task.</li> <li>- Integrate Nextflow with HPC resources: Modify a Nextflow workflow for an HPC cluster.</li> <li>- Data pipelines for machine learning: Create a data pipeline for ML data preprocessing.</li> <li>- Distributed computing with Dask: Design a Dask computation for distributed computing.</li> <li>- Enhance Nipype workflow with custom interfaces: Extend a Nipype workflow with custom interfaces.</li> <li>- Data pipeline optimization challenge: Identify and optimize a pipeline bottleneck.</li> <li>- Data provenance and reproducibility: Implement data provenance tracking in a pipeline.</li> <li>- Error handling and resilience in pipelines: Introduce errors and implement error handling strategies.</li> <li>- Introduction to Deep Learning: <ul style="list-style-type: none"> <li>- Definition and significance in modern machine learning.</li> <li>- Brief historical overview.</li> </ul> </li> </ul>
	26 Hands-on session	
	27 Foundations of Deep Learning	<ul style="list-style-type: none"> <li>- Neural Network Basics: <ul style="list-style-type: none"> <li>- Detailed discussion on neural network architecture.</li> <li>- Explanation of layers, neurons, and their interconnections.</li> <li>- Activation functions and their role in introducing non-linearity.</li> <li>- Illustration of forward and backward passes in a neural network.</li> </ul> </li> <li>- Overview of the training process in deep learning.</li> <li>- The role of data in supervised learning.</li> <li>- The importance of differentiability and its role in optimization</li> </ul>
	28 Training Deep Neural Networks	<ul style="list-style-type: none"> <li>- Training Deep Neural Networks and key training concepts: <ul style="list-style-type: none"> <li>- Batches: Definition, significance, and impact on training.</li> <li>- Epochs: Understanding the concept of one complete pass through the entire dataset.</li> <li>- Learning rate: Importance, tuning strategies, and common challenges.</li> <li>- Loss functions: Overview and selection based on task.</li> </ul> </li> <li>- DL frameworks: TensorFlow, PyTorch, Keras, etc.</li> </ul>
8	29 Introduction to PyTorch Fundamentals	<ul style="list-style-type: none"> <li>- Overview of PyTorch and its role in deep learning.</li> <li>- Installation and setup of PyTorch.</li> <li>- Introduction to PyTorch tensors and basic operations.</li> <li>- Building a simple neural network using PyTorch.</li> <li>- Exploring PyTorch modules and autograd for automatic differentiation.</li> <li>- Defining and training more complex neural network architectures.</li> <li>- Guided exercises to reinforce PyTorch fundamentals.</li> <li>- Discussion on best practices for PyTorch development.</li> <li>- Debugging with PyTorch: gathering, understanding and processing failure evidence</li> </ul>
	30 Deepening PyTorch Concepts	
	31 PyTorch for Computer Vision and Natural Language Processing	<ul style="list-style-type: none"> <li>- Introduction to PyTorch's torchvision and torchaudio libraries.</li> <li>- Building and training models for computer vision tasks.</li> <li>- Utilizing pre-trained models for transfer learning.</li> <li>- Basic natural language processing tasks using PyTorch.</li> </ul> <p>Student 1: Monitoring Training in PyTorch</p> <ul style="list-style-type: none"> <li>- Explore different techniques for monitoring and visualizing training progress in PyTorch.</li> <li>- Discuss the use of TensorBoard, PyTorch Ignite and Lightning, and</li> <li>- Present best practices for tracking metrics, loss curves, and model performance during training.</li> </ul>
	32 "Changing hats" session (PyTorch)	<p>Student 2: Transfer Learning with PyTorch</p> <ul style="list-style-type: none"> <li>- Provide an in-depth overview of transfer learning techniques using PyTorch.</li> <li>- Discuss pre-trained models, feature extraction, and fine-tuning strategies.</li> <li>- Demonstrate how to implement transfer learning on a practical project or dataset.</li> </ul> <p>Student 3: Convolutional Networks in PyTorch</p> <ul style="list-style-type: none"> <li>- Dive into the fundamentals of convolutional neural networks (CNNs) in PyTorch.</li> <li>- Explain the architecture of a basic CNN and its components (convolutional layers, pooling layers).</li> <li>- Walk through the implementation of a simple image classification task using a CNN in PyTorch.</li> </ul>

Week	Lectur Title	Contents
9	33 Consolidate "changing hats" session	<ul style="list-style-type: none"> <li>- Consolidate the changing hats session: <ul style="list-style-type: none"> <li>- Briefly recap the key points covered by each student in the previous Changing Hats session.</li> <li>- Discuss difficult points and bring up elements that were not covered in sufficient depth or with clarity</li> </ul> </li> <li>- Introduction to Transfer Learning <ul style="list-style-type: none"> <li>- Definition and motivation behind transfer learning.</li> <li>- Explanation of pre-trained models and their role in transfer learning.</li> <li>- Demonstration of how to implement transfer learning in PyTorch.</li> </ul> </li> </ul>
	34 Hands-on: peer-programming	<ul style="list-style-type: none"> <li>- Distributed Hyperparameter Optimization in PyTorch with Ray Tune</li> <li>- Implement a simple CNN for image classification using the CIFAR-10 dataset.</li> <li>- Apply transfer learning with a pre-trained CNN for image classification.</li> <li>- Develop an RNN for text classification using a small or synthetic dataset.</li> <li>- Extend an image classification project to incorporate data parallelism.</li> <li>- Generate images using a GAN and implement model parallelism for efficiency.</li> <li>- Combine transfer learning and model parallelism for image classification.</li> <li>- Implement an RNN for time series prediction using synthetic or real data.</li> <li>- Apply data parallelism to a regression task and compare performance.</li> <li>- Create an image captioning model using a sequence-to-sequence architecture.</li> <li>- Implement model parallelism in a project tailored to a custom dataset.</li> </ul>
	35 Parallel programming on HPC requiring GPU resources	<ul style="list-style-type: none"> <li>- (Big) Data and Model Size - Why Distributing the Workload? <ul style="list-style-type: none"> <li>- Explore the challenges posed by large datasets and complex models in traditional computing environments.</li> <li>- Understand the need for distributing workloads to efficiently process extensive data and intricate models.</li> <li>- Discuss the limitations of sequential processing and how parallelization can address these challenges.</li> </ul> </li> <li>- Parallelization Within a Node with Several GPUs <ul style="list-style-type: none"> <li>- Dive into the architecture of a single computing node equipped with multiple GPUs.</li> <li>- Explore techniques for parallelizing computations within a node, leveraging the parallel processing capabilities of individual GPUs.</li> <li>- Understand the nuances of load balancing and optimizing performance when multiple GPUs collaborate within a single node.</li> </ul> </li> <li>- Parallelization Across GPU Nodes <ul style="list-style-type: none"> <li>- Extend the discussion to parallelization across multiple nodes, forming a distributed GPU computing environment.</li> <li>- Examine the communication challenges and strategies for coordinating computations across GPU nodes.</li> <li>- Discuss frameworks and libraries that facilitate distributed GPU computing, ensuring efficient parallel processing at scale.</li> </ul> </li> <li>- Student 1: Diving into MPI, OpenMP, and CUDA for parallelization <ul style="list-style-type: none"> <li>- Present the implementation of a parallelized algorithm using MPI for distributed computing.</li> <li>- Explain shared-memory parallelization using OpenMP on an HPC node.</li> <li>- Showcase GPU-accelerated code using CUDA for efficient parallel processing.</li> <li>- Mention challenges and considerations in parallelizing algorithms with different frameworks.</li> </ul> </li> </ul>
	36 Changing hats: HPC parallelization	<ul style="list-style-type: none"> <li>- Student 2: Parallelization with TensorFlow <ul style="list-style-type: none"> <li>- Present the implementation of a parallel machine learning model using TensorFlow.</li> <li>- Explain distributed training strategies with TensorFlow.</li> <li>- Discuss optimization techniques for parallelizing computations in TensorFlow.</li> <li>- Enumerate some challenges and best practices in parallelizing deep learning models.</li> </ul> </li> <li>- Student 3: Parallelization with PyTorch <ul style="list-style-type: none"> <li>- Present the implementation of a parallel machine learning model using PyTorch.</li> <li>- Explain PyTorch's native support for parallel computing.</li> <li>- Discuss strategies for optimizing and scaling PyTorch-based applications.</li> </ul> </li> </ul>
10	37 Consolidate "changing hats" session	<ul style="list-style-type: none"> <li>- Consolidate the changing hats session: <ul style="list-style-type: none"> <li>- Briefly recap the key points covered by each student in the previous Changing Hats session.</li> <li>- Discuss difficult points and bring up elements that were not covered in sufficient depth or with clarity</li> </ul> </li> <li>- Describe the reasons to distribute machine learning models: <ul style="list-style-type: none"> <li>- Sizing the problem dimensions (data volume and model size)</li> <li>- Privacy/security/access</li> <li>- Examples: model ensembles and federated learning.</li> </ul> </li> <li>- Understanding what can be parallelized: <ul style="list-style-type: none"> <li>- Model training: distributing the workload across multiple devices or nodes</li> <li>- Model inference: parallelizing the prediction process</li> <li>- Data processing: expedite model training by parallelizing feature extraction and engineering</li> </ul> </li> <li>- Challenges of parallelizing ML applications: complexity, I/O overhead, synchronization, data consistency, scalability, fault tolerance.</li> <li>- Monitoring in HPC - introduction and tools <ul style="list-style-type: none"> <li>- Explain the critical role of monitoring in ensuring the efficiency, reliability, and performance of HPC systems.</li> <li>- Discuss the impact of monitoring on resource utilization, fault detection, and overall system health.</li> <li>- Introduce popular monitoring tools in HPC, such as Ganglia, Nagios, and Prometheus.</li> <li>- Discuss key metrics for monitoring, including CPU utilization, memory usage, network traffic, and disk I/O.</li> <li>- Relevance of real-time monitoring for identifying bottlenecks and optimizing resource allocation.</li> <li>- Live Demonstration using a monitoring tool to showcase real-time data visualization and analysis on DISCO</li> </ul> </li> </ul>
	38 Monitoring and Control of HPC, with a focus on distributed ML models	<ul style="list-style-type: none"> <li>- Monitoring Distributed ML Models on HPC <ul style="list-style-type: none"> <li>- Challenges in Monitoring ML Workloads</li> <li>- Monitoring Frameworks for ML Models, such as TensorFlow's TensorBoard and PyTorch's built-in monitoring capabilities.</li> <li>- Discuss the integration of these frameworks with HPC systems for comprehensive monitoring.</li> </ul> </li> <li>- Case Study highlighting the successful implementation of monitoring strategies for distributed ML models on HPC.</li> </ul>
	39 PyTorch's distributed package	<ul style="list-style-type: none"> <li>- Control and Optimization Strategies <ul style="list-style-type: none"> <li>- Dynamic Resource Allocation: introduction and tools</li> <li>- Discuss how monitoring data can inform adjustments to hyperparameters for optimal model performance.</li> </ul> </li> <li>- Overview of PyTorch distributed AI capabilities <ul style="list-style-type: none"> <li>- Introduce DDP, RPC, and c10d</li> <li>- Recap of data parallelism and its applications</li> <li>- Recap of model parallelism and its applications</li> <li>- Recap of inference parallelism and its applications</li> </ul> </li> </ul>
	40 Data parallelism in PyTorch	<ul style="list-style-type: none"> <li>- Running single-machine, multi-GPU DataParallel and the role of CUDA parallelizing data splits</li> <li>- Running multi-machine DistributedDataParallel to scale across nodes</li> <li>- Introduce how the model is kept synchronized across workers that are training on different data splits</li> <li>- Introduce "sharding" and the FullyShardedDataParallel training</li> </ul>
11	41 Model parallelism in PyTorch	<ul style="list-style-type: none"> <li>- Running simple PyTorch models with several GPUs in parallel</li> <li>- Pipelining inputs to optimize model parallelization</li> <li>- Pipeline parallelism using multiple GPUs (torch.distributed.pipeline)</li> <li>- Model parallelism across compute nodes - introduction to the Distributed RPC framework</li> </ul>
	42 Data & model parallelism in PyTorch	<ul style="list-style-type: none"> <li>- Consolidate the concepts of the two previous lectures</li> <li>- Introduce torch.distributed.elastic for fault-tolerant and dynamic allocation training</li> <li>- Mixed-precision training using torch.cuda.amp</li> <li>- Gradient accumulation for larger effective batch sizes</li> <li>- Wrap-up overview of distributed training</li> <li>- Explore paramount real-world examples of parallel techniques for training large models</li> </ul>
	43 Parallelizing inference in PyTorch	<ul style="list-style-type: none"> <li>- CPU parallelization</li> <li>- GPU parallelization</li> <li>- Edge devices and distributed inference</li> <li>- Federated learning as a combination of large models that require parallelization and AI on edge devices</li> <li>- Create and run a simple PyTorch model on a single machine with multiple GPUs using DataParallel.</li> <li>- Create and run a simple PyTorch model using DistributedDataParallel across multiple machines.</li> <li>- Implement a mechanism to keep a model synchronized across workers training on different data splits.</li> <li>- Experiment with sharding techniques and implement FullyShardedDataParallel training.</li> <li>- Run a PyTorch model on a machine with several GPUs in parallel, exploring GPU parallelization.</li> <li>- Implement input pipelining techniques to optimize model parallelization.</li> <li>- Extend model parallelism to operate across compute nodes, using the Distributed RPC framework.</li> <li>- Introduce and experiment with torch.distributed.elastic for fault-tolerant training</li> <li>- Implement mixed-precision training on an existing model using torch.cuda.amp for faster computation.</li> <li>- Experiment with gradient accumulation techniques to achieve larger effective batch sizes, optimizing training efficiency.</li> </ul>
	44 Hands-on session: PyTorch	
	45 Generalizability of Inference and Domain Shifts	<ul style="list-style-type: none"> <li>- Definitions and background: generalizability and domain shift</li> <li>- Sources of bias that set boundaries to generalizability</li> <li>- The relationship between the training dataset and biases</li> <li>- Mitigating biases and ensuring the diversity and representativeness of the dataset</li> <li>- Algorithmic fairness and ethical implications</li> </ul>

Week	Lectur Title	Contents
12	46 Cross-Validation and Nested Cross-Validation	<ul style="list-style-type: none"> <li>- Re-introduce cross-validation as a robust model evaluation technique</li> <li>- K-fold cross-validation</li> <li>- Stratification and operation on "imbalanced datasets"</li> <li>- Nested cross-validation for robust model selection and evaluation</li> <li>- Model selection as a source of bias</li> <li>- Showcase examples where nested cross-validation demonstrates model selection biases</li> <li>- Batch-effects (genomics), site-effects (other fields)</li> </ul>
	47 Domain Adaptation and Transfer Learning	<ul style="list-style-type: none"> <li>- Briefly recap theory on generalizability and domain shifts</li> <li>- Zero-shot learning, domain generalization, test-time adaptation and examples</li> <li>- Objectives of domain adaptation</li> <li>- Adversarial training as a technique for domain adaptation by minimizing domain discrepancy</li> <li>- Concept of task, multi-task learning, and lifelong learning</li> <li>- Transfer learning: practical implementation</li> </ul>
	48 Transfer Learning with PyTorch	<ul style="list-style-type: none"> <li>- Navigate the pre-trained models available within torchvision and their applications</li> <li>- Investigate fine-tuning procedures using PyTorch</li> <li>- Tutorial: transfer learning of a torchvision model</li> </ul>
13	49 Generative Models 1	<ul style="list-style-type: none"> <li>- From discriminative to generative models.</li> <li>- Introduce probabilistic graphical models as a foundation for generative models. <ul style="list-style-type: none"> <li>- Latent variables</li> </ul> </li> <li>- Classical generation: energy-based models (EBMs)</li> <li>- Generative Adversarial Networks (GANs) <ul style="list-style-type: none"> <li>- Adversarial training process in depth</li> </ul> </li> </ul>
	50 Generative Models 2	<ul style="list-style-type: none"> <li>- Explore Variational Autoencoders (VAEs) and their use in generative modeling. <ul style="list-style-type: none"> <li>- Encoder-decoder architectures</li> </ul> </li> <li>- Flow-based generative models and differences with VAEs and GANs</li> <li>- Autoregressive models (ARMs)</li> <li>- Showcase applications of generative models in image synthesis, text generation, etc.</li> </ul>
	51 Transformers	<ul style="list-style-type: none"> <li>- Precedents: Recurrent Neural Networks, long short-term memory (LSTM) networks</li> <li>- Introducing ML attention <ul style="list-style-type: none"> <li>- Implementation of the self-attention mechanism</li> </ul> </li> <li>- Transformers and their revolutionary impact on natural language processing.</li> <li>- Architecture of transformers: <ul style="list-style-type: none"> <li>- Encoder-decoder and attention layers</li> </ul> </li> <li>- Application of transformers on NLP</li> </ul>
	52 Graph Learning	<ul style="list-style-type: none"> <li>- Introduction to graph learning and the model representation of graph data</li> <li>- Foundations of graph neural networks (GNNs) <ul style="list-style-type: none"> <li>- Message passing and other GNNs operations</li> </ul> </li> <li>- Showcase social network analyses</li> </ul>
14	53 Diffusion Models	<ul style="list-style-type: none"> <li>- Recap of flow-based models seen in lecture 50</li> <li>- Diffusion models and their fundamental principles.</li> <li>- Stochastic processes and how diffusion models capture data evolution.</li> <li>- Explore how diffusion models can be applied to denoise images and image restoration.</li> <li>- Super-resolution, its importance in image processing, and its implementation with diffusion models</li> <li>- Introduce latent diffusion as a powerful approach for generative modeling.</li> </ul>
	54 Topic hold and/or Advanced optimizations and tools	<ul style="list-style-type: none"> <li>- Recover topics that may require an additional recap</li> <li>- Mention torch_xla to execute PyTorch on XLA devices (e.g., TPUs)</li> <li>- Introduce torch.cuda.amp to implement mixed-precision training</li> <li>- Introduce Google's JAX</li> <li>- Wandb (weights &amp; biases) developer platform</li> </ul>
	55 Hands-on sessions	<ul style="list-style-type: none"> <li>- Dataset audit: find biases in openly available datasets</li> <li>- Using pre-processing techniques to mitigate biases in a given dataset.</li> <li>- Document ethical implications related to biases in machine learning.</li> <li>- Implement K-fold cross-validation on a dataset for model evaluation.</li> <li>- Apply stratification techniques for handling imbalanced datasets.</li> <li>- Perform nested cross-validation for robust model selection and evaluation.</li> <li>- Investigate examples showcasing biases in model selection using nested cross-validation.</li> <li>- Explore batch-effects in genomics and site-effects in other fields.</li> <li>- Implement transfer learning using pre-trained models from torchvision.</li> <li>- Fine-tune a pre-trained torchvision model using PyTorch for a specific task.</li> </ul>
	56 Federated Learning (FL) 1	<ul style="list-style-type: none"> <li>- Significance of FL in the context of distributed machine learning.</li> <li>- Discuss the motivation behind FL and its applications.</li> <li>- Contrast centralized vs. decentralized learning approaches.</li> <li>- Training models on decentralized devices</li> <li>- Components and their communication: server, clients, and FL algorithm</li> <li>- Privacy concerns in traditional machine learning models.</li> <li>- Keeping data local: privacy-preserving applications.</li> <li>- Secure aggregation techniques</li> <li>- Applications on healthcare, finance, and edge computing</li> </ul>
15	57 FL 2	<ul style="list-style-type: none"> <li>- Optimization techniques specific to FL.</li> <li>- Reducing communication overhead with quantization and sparsification</li> <li>- Ultra-light DNN architectures</li> <li>- FL frameworks (e.g., TensorFlow Federated, PySyft).</li> <li>- Federated averaging and model aggregation.</li> <li>- Challenges: non-IID data, communication bottlenecks, and model heterogeneity.</li> <li>- Technical limitations</li> </ul>
	58 Tutorial: implementing FL with PySyft	<ul style="list-style-type: none"> <li>- PySyft and its purpose in the context of FL.</li> <li>- Installation and compatibility with PyTorch</li> <li>- PySyft workers: concept, initialization and communication</li> <li>- Secure multi-party computation, encrypted tensors, and computation on encrypted data</li> <li>- Showcase an application using PySyft</li> </ul>
	59 Advanced Topics in Distributed AI	<ul style="list-style-type: none"> <li>- Apply reinforcement learning concepts to distributed scenarios.</li> <li>- Discuss emergent behavior in multi-agent systems.</li> <li>- Explore how local interactions lead to global patterns.</li> <li>- Explore emerging trends in distributed AI such as edge computing</li> </ul>
	60 Exam preparation	<ul style="list-style-type: none"> <li>- A sessions where students can ask questions about the contents and about the exam</li> <li>- Some parts of the exam will be hinted, so that the students can understand the priorities over the content</li> </ul>
16	61 Invited lecture	Fabian Pedregosa (JAX, Google Inc) or Chris Gorgolewski (Bard, Google Inc.)
	62 Exam	
	63 Exam revision	
	64 Recap and evaluation	<ul style="list-style-type: none"> <li>- Open format where students can ask about any of the contents seen over the course</li> </ul>