Transfer Learning Workflow for I/O Bandwidth Prediction

HPC I/O in the Data Center Workshop 2023

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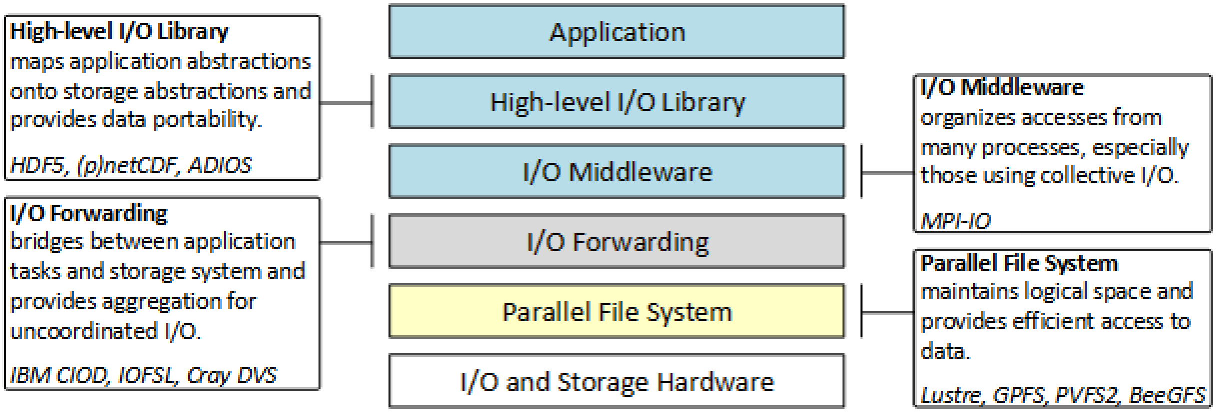
Background & motivation

Why should we predict the I/O bandwidth of the jobs on the cluster?

- Useful for optimizing performance & efficiency
  - Identify performance anomalies
  - Tune the filesystem
  - Make better hardware procurement decisions
  - Potentially implement hardware optimizations (lower energy usage etc.)



Extracted from [1]

- BUT requires a lot of data from the specific cluster
  - Need to set up a monitoring & processing pipeline
  - Takes a lot of time to collect a significant amount

Background & motivation

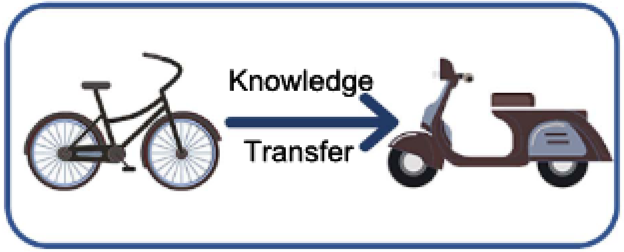
Transfer Learning for I/O Prediction

- Relies on the assumption that „different clusters might exhibit similar I/O characteristics“
  - Same filesystems
  - Same I/O APIs such as POSIX, MPI-IO, etc.
  - Similar applications (e.g. computational fluid dynamics or biomedical simulations)

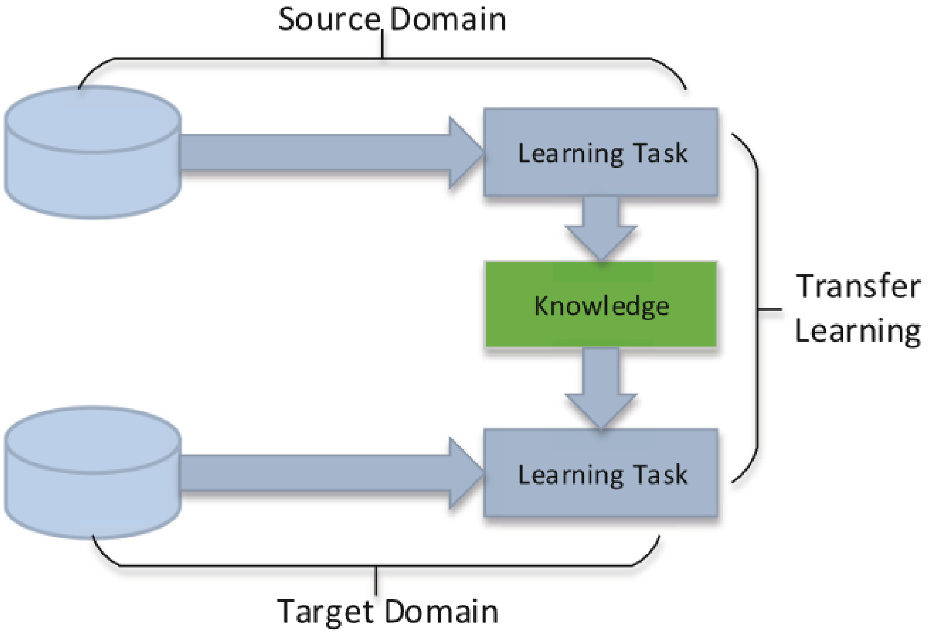
- Use an already existing dataset from another cluster
  - Years of I/O performance data
  - Real-life application runs

- Fine-tune on a small dataset collected at the target installation
  - Relatively short time to gather the data
  - Might work as a Proof-of-Concept for hardware procurement

Transfer Learning: The Idea



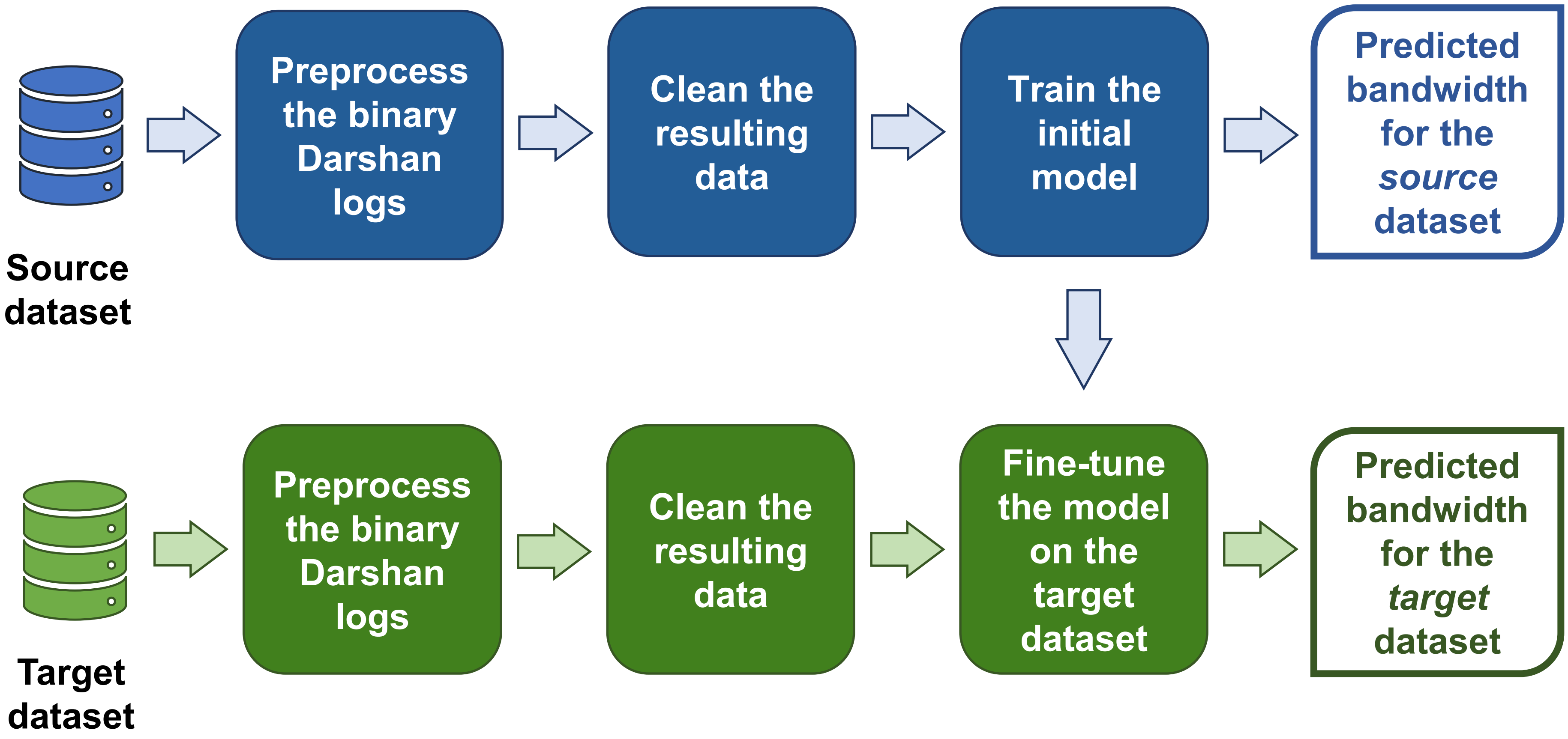
Extracted from [2]



Extracted from [3]

Try to predict the I/O bandwidth of a specific job on a specific cluster, based on the observations from another cluster

Proposed workflow

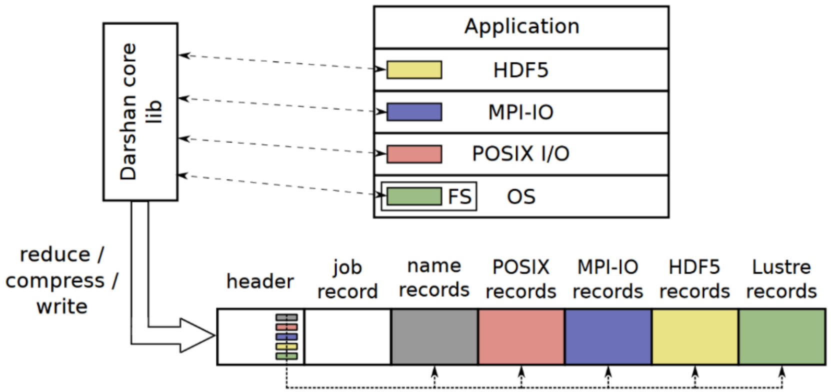


Preprocessing the binary Darshan logs

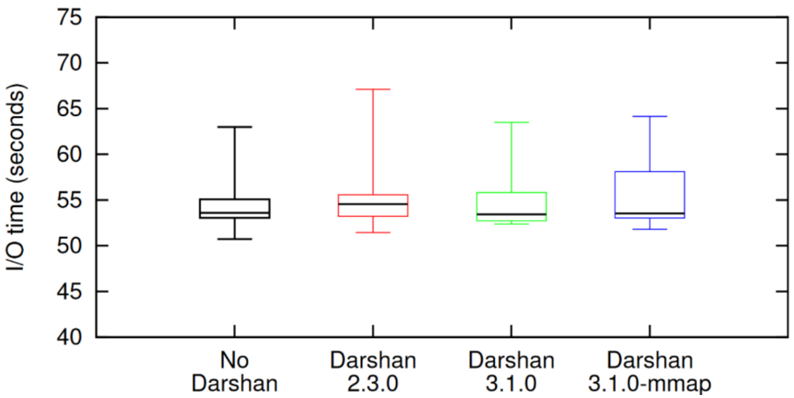
Why Darshan?

- Developed at the Argonne National Lab
- A well-known tool for the I/O performance measurement & shown to be reliable
- Minimal influence on the applications‘ I/O time (less than 3% [19])
- Binary log format allows storing significant amounts of performance data

- Several large-scale public datasets are already available



Overview of Darshan’s architecture & log format [14]



Darshan’s influence on I/O time of the instrumented application [14]

Preprocessing the binary Darshan logs

Prediction target design

- Focus on the POSIX module for now
  - De facto standard for I/O operations on Unix-like filesystems
  - MPI-IO, HDF5, and other APIs are implemented on top of it
    - Their calls are reflected in the corresponding POSIX ops counters [18]
  - Potentially more data, as using MPI-IO requires POSIX, but not vice versa [18]
  - Existing body of work to compare against

- Parse the binary logs using PyDarshan
  - Python module from the authors of Darshan
  - Provides a summary of sizes, times, the I/O histogram, and so on

  - Does not calculate the bandwidth by default → must be done separately

Preprocessing the binary Darshan logs

Datasets (both collected at the Lustre filesystem)

- **Blue Waters (source dataset)**
  - Gathered during 2012-2021 at the University of Illinois
  - More than 4.65 mln individual files
  - The subset used contains ~690k records
    - Not all logs contain POSIX performance data
    - PyDarshan supports only logs recorded with v3.21+

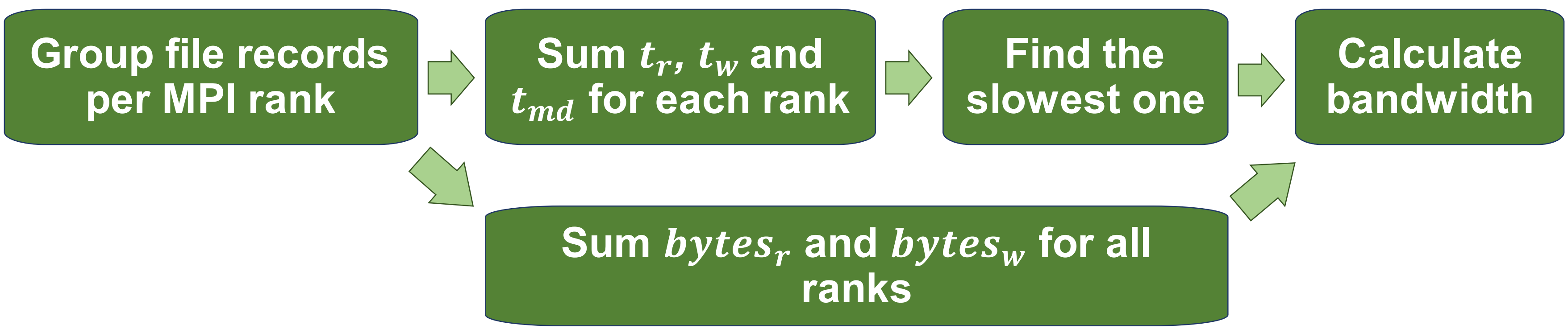
- **CLAIX (target dataset)**
  - Data from several applications:
    - C-Class NAS Parallel Benchmark from NASA
      - 4, 9, 16, 64-process variants
    - Ciao - 48, 144, 162, 240 processes
    - Quantum Espresso was considered, but removed due to the very high variance it introduced
  - Limited size

Preprocessing the binary Darshan logs

How to calculate the bandwidth?

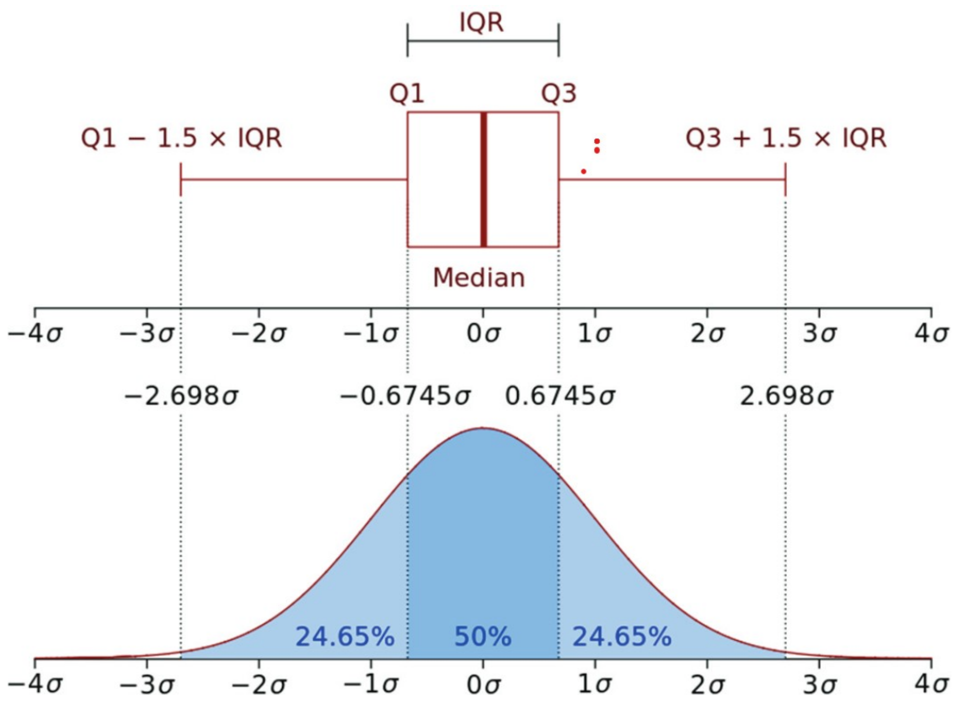
$$MiB/s = \left(\frac{\sum_{rank=0}^{n-1} (bytes_r + bytes_w)}{\max_{rank=0}^{n-1} (t_{md} + t_r + t_w)} \right)$$

Darshan’s bandwidth formula [14]



Bandwidth calculation workflow for an individual Darshan log

Cleaning the resulting data



The IQR and its projection on a normally distributed density [15]

- High number of outliers causes problems with model convergence
  - Three-stage removal process
    - Eliminate erroneous items, e.g., with negative times (similar to [18])
    - Remove all-zero features
    - Apply the Interquartile Range (IQR) method to the rest

What is the input?

Darshan job summary (by PyDarshan)

- 96 different POSIX counters + **# of processes:**
  - **Times:**
    - POSIX_F_READ_TIME, POSIX_F_WRITE_TIME …
    - POSIX_F_SLOWEST_RANK_TIME …
  - **Sizes:**
    - POSIX_BYTES_WRITTEN, POSIX_BYTES_READ
    - POSIX_SLOWEST_RANK_BYTES, POSIX_FASTEST_RANK_BYTES
    - 4 most frequently appearing **access** sizes & **strides**
  - **Ops counts:**
    - POSIX_OPENS, POSIX_SEEKS, POSIX_STATS …
    - POSIX_CONSEC_READS, POSIX_CONSEC_WRITES …
    - 4 most frequently appearing **access** sizes & **strides**
  - **I/O histogram**
    - Number and total size of read/write ops split into brackets:
      - 0-100B, 100B-1KB, …, 1GB+
  - **Alignments (file & memory)**
  - **Read/write switches**
  - **POSIX mode**
  - **Offsets etc.**

Training the source model

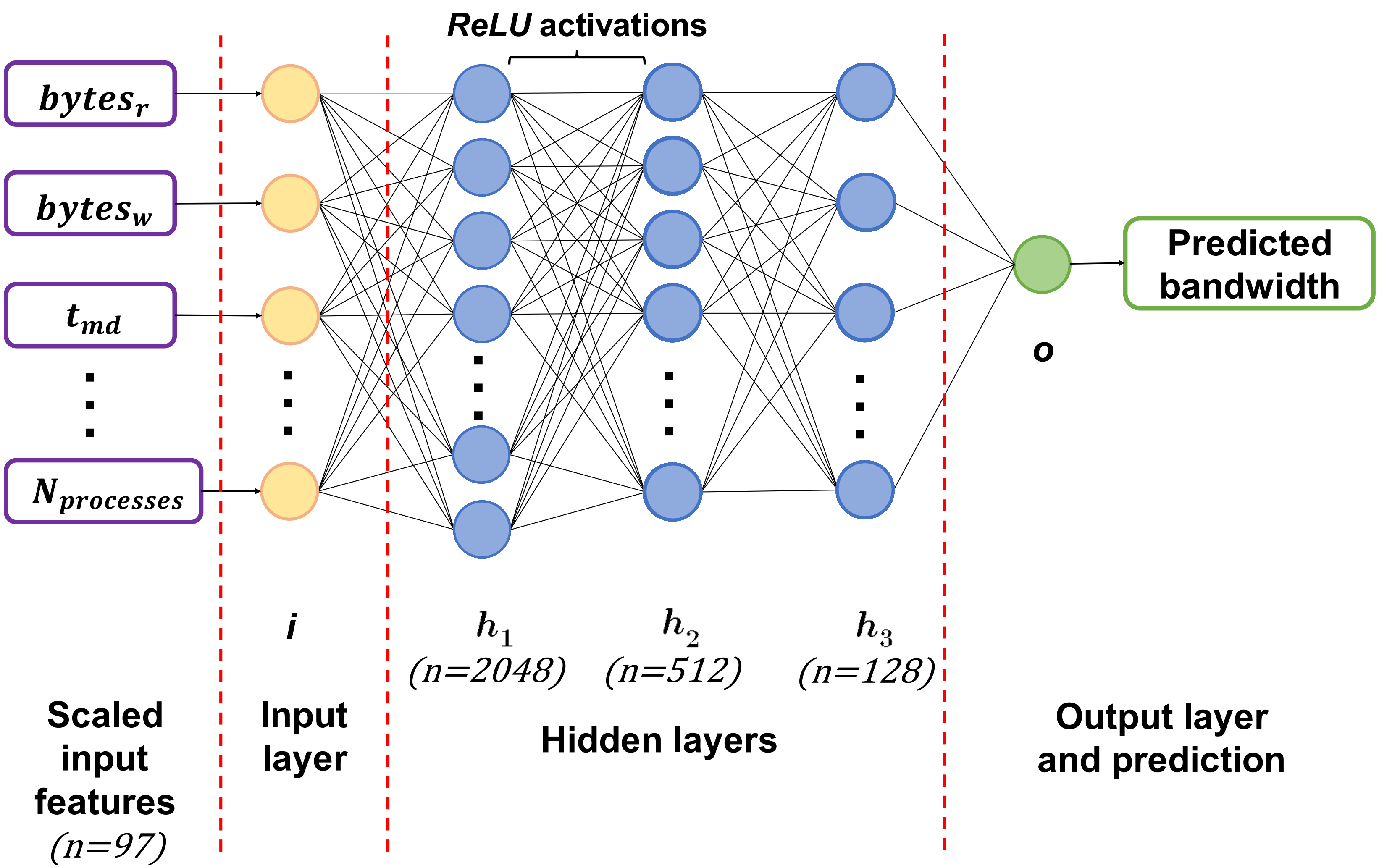
- Architecture: Multi-Layer Perceptron
  - Mathematically proven universal approximator [16]
  - No structure of the features to rely on for a CNN
  - No time series → not well-suited for an RNN

  - Efficient: total time to train ~60 mins

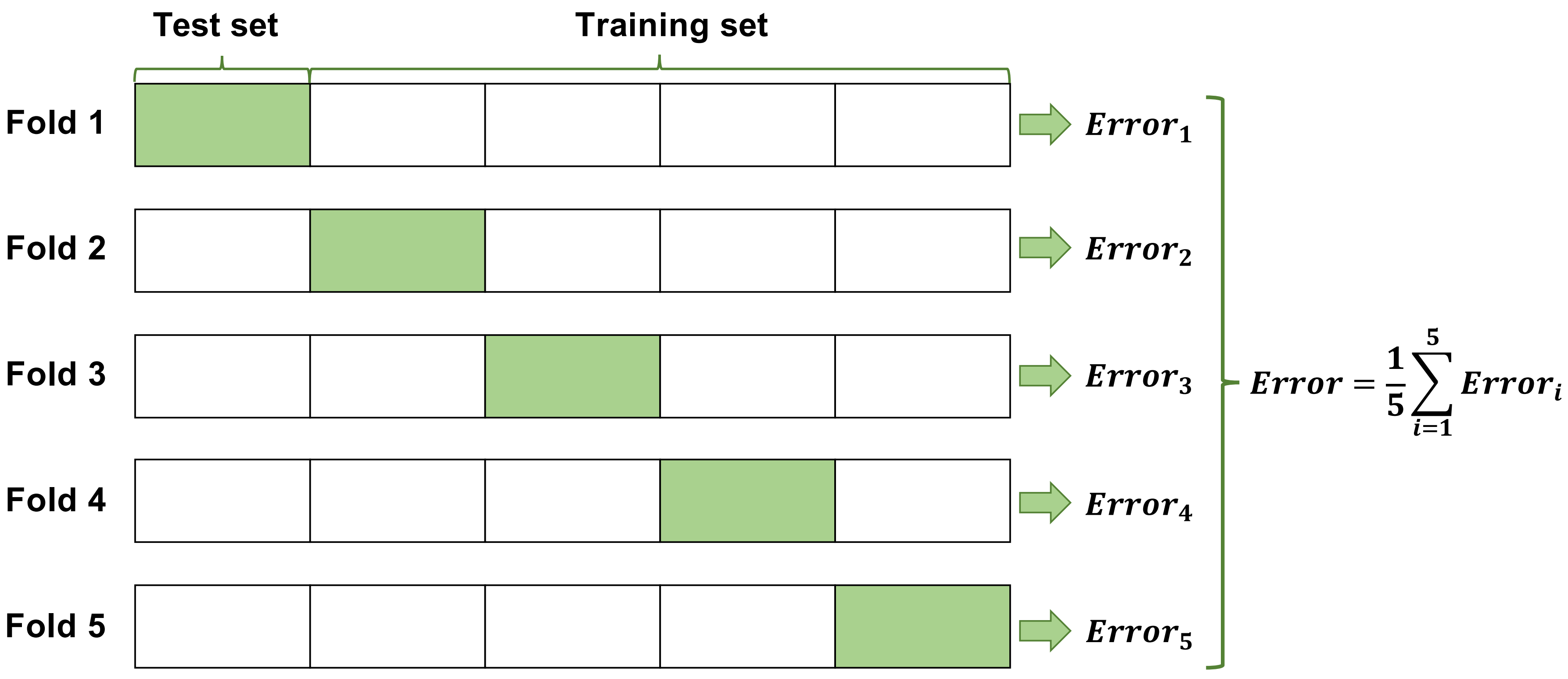
- 2 different sets of the training data:
  - Full dataset
  - Subset with the number of processes per job that appears at least once in the target data

  - Motivation: some of the jobs in the Blue Waters dataset would be physically impossible to run on the CLAIX cluster
    - The model does not need to generalize to them
    - Try to focus on more realistic data → potentially better performance

Neural network architecture

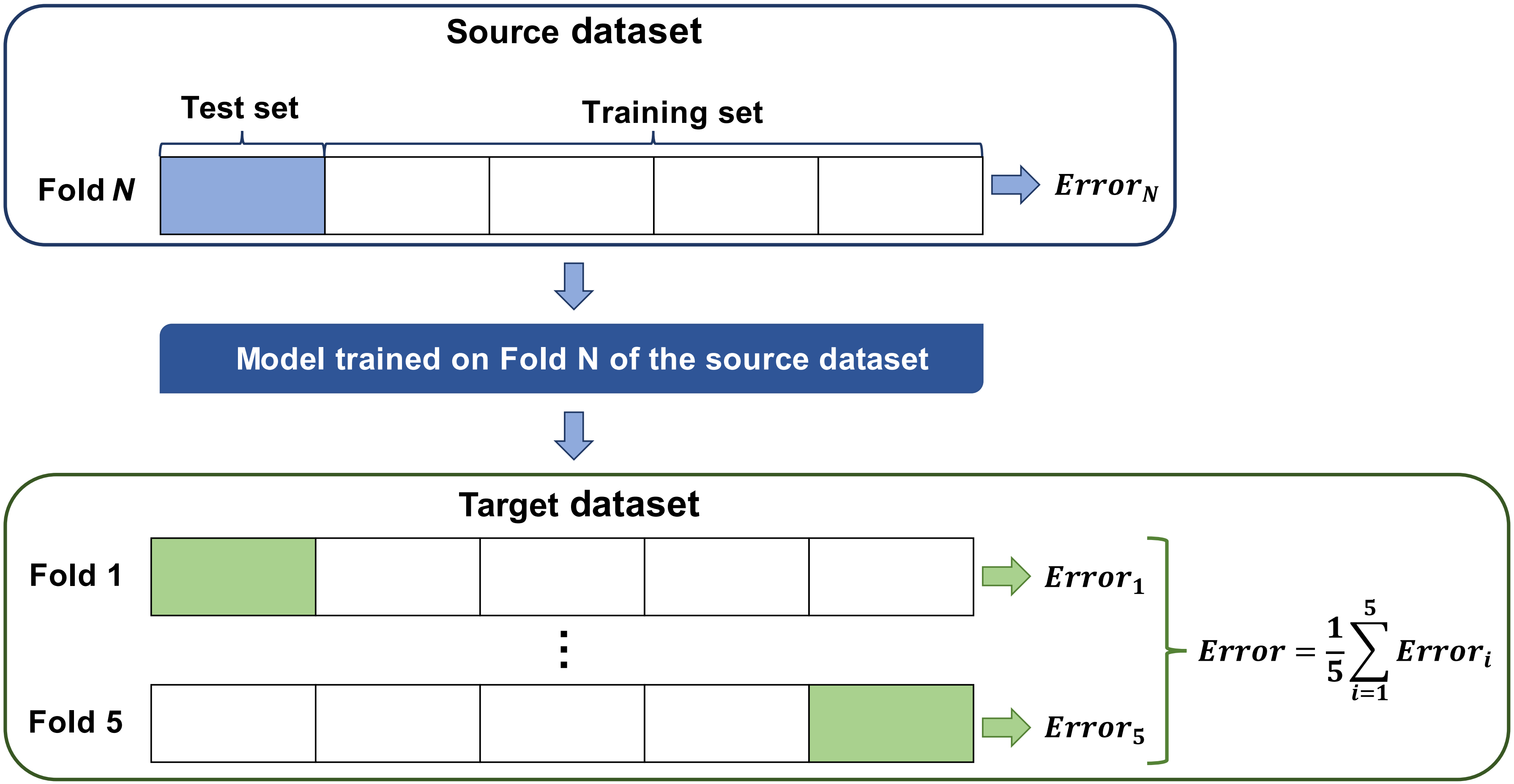


Validating the results – Initial training



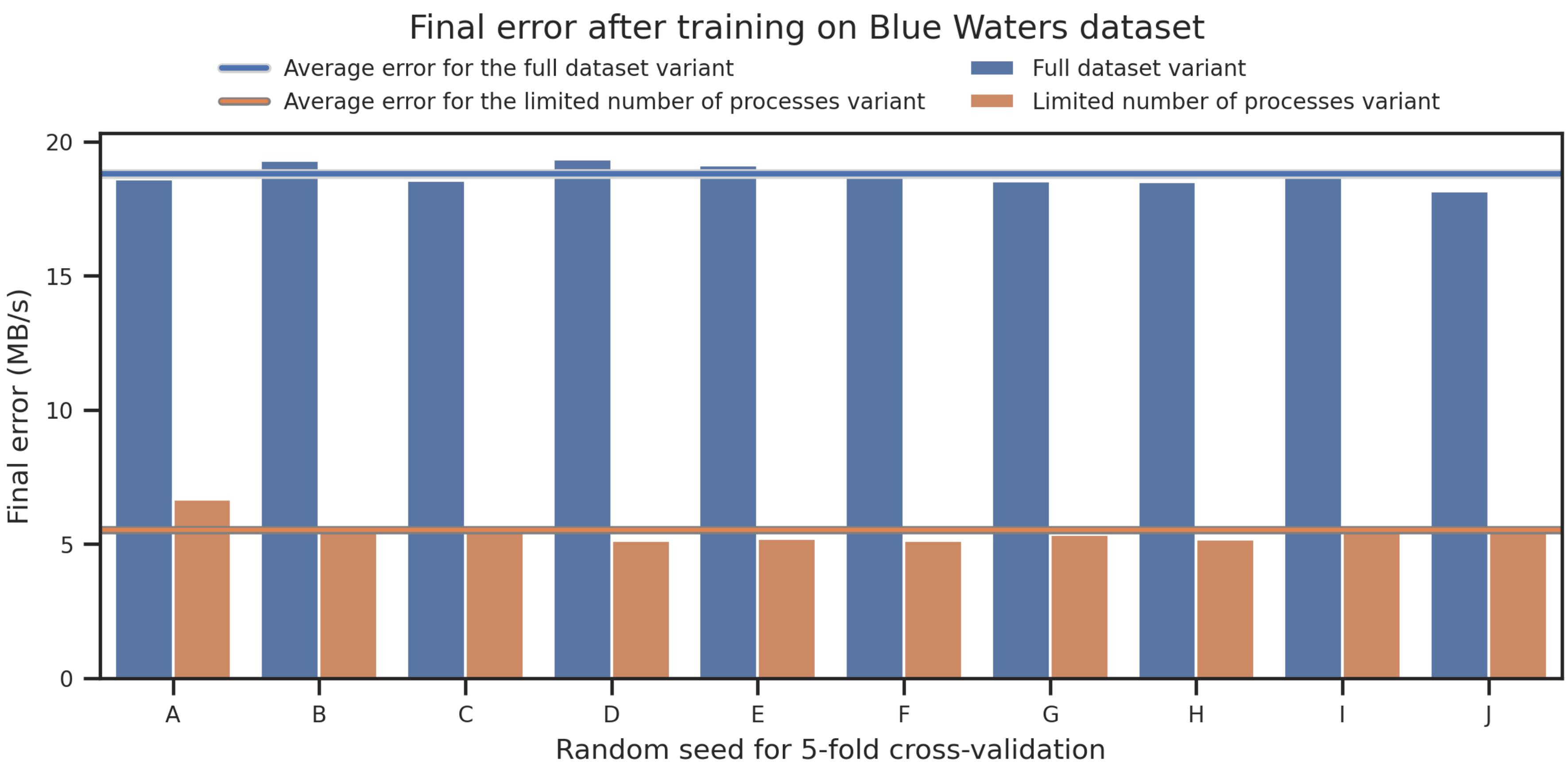
The principle of 5-fold cross-validation

Validating the results – Transfer learning



Cross-validation of the transfer learning

Results of the initial training on the Blue Waters dataset



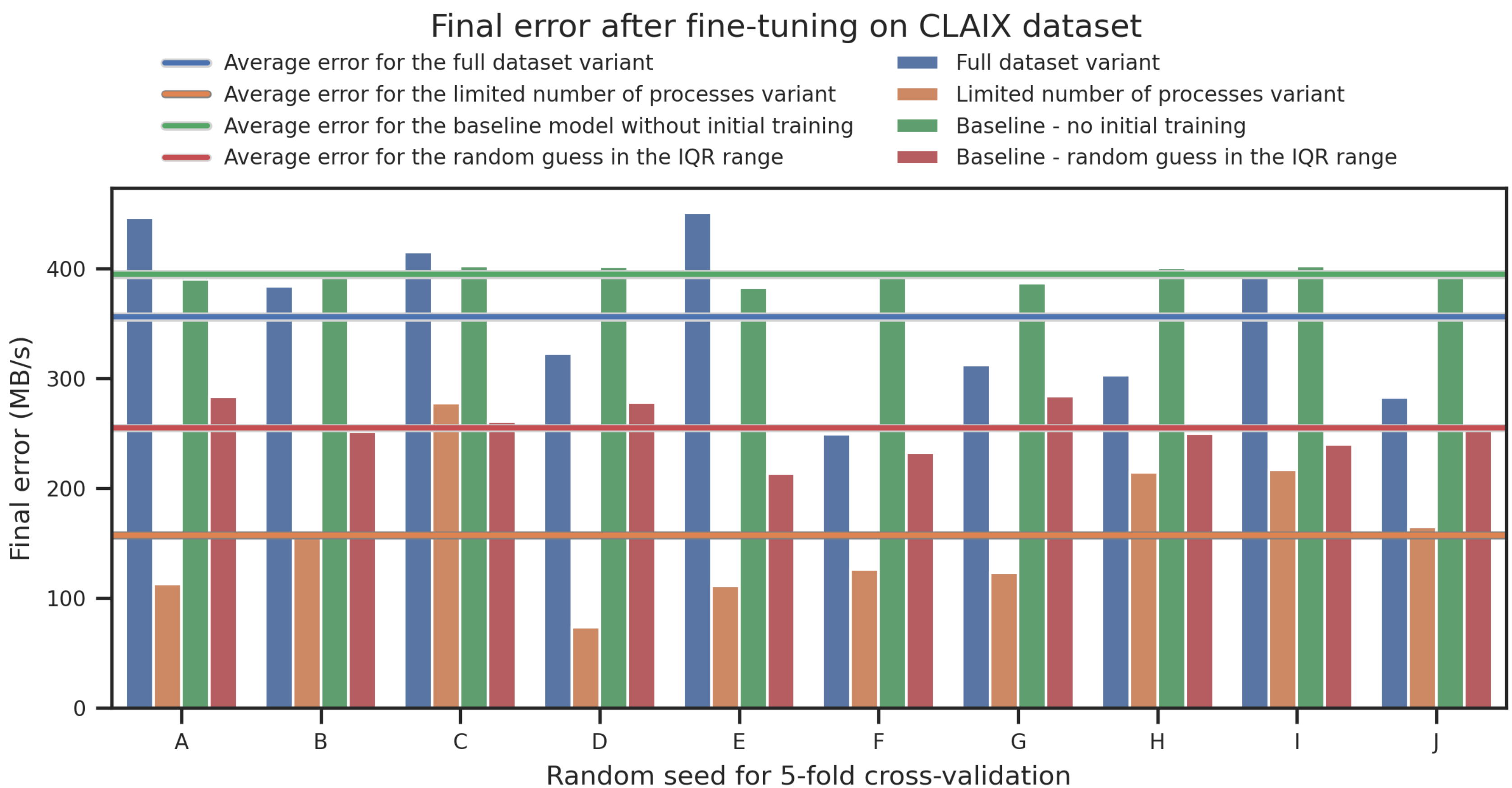
Variant	Full dataset	Limited # of processes	Random guess in IQR
MAE (*n=50*)	18.81 MB/s	**5.53 MB/s**	155.4 MB/s

Fine-tuning the model

- All models were fine-tuned using the same network-based transfer learning setup
  - Weights of the output layer reset
  - All layers unfrozen
  - Trained for 1200 epochs (vs 600 on the source dataset)

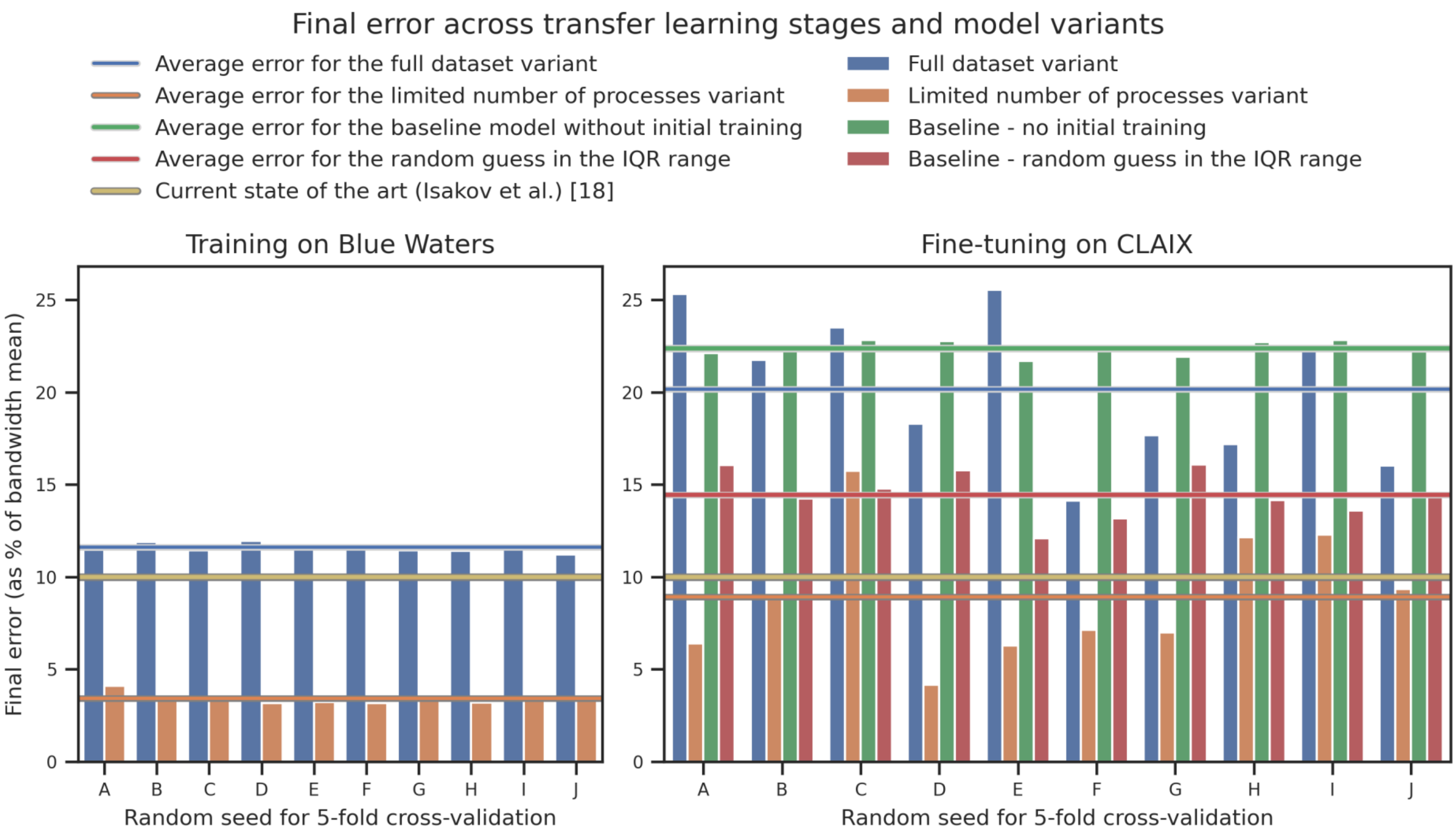
  - Fine-tuning time: <1 min on P100 GPU, ~6 mins on an Intel CPU
    - Very low resource requirements

Results after fine-tuning on the data from CLAIX



Variant	Full dataset	Limited # of processes	No initial training	Random guess in IQR
MAE	355.92 MB/s	**157.44 MB/s**	394.67 MB/s	254.75 MB/s

Comparison of results between the transfer learning stages

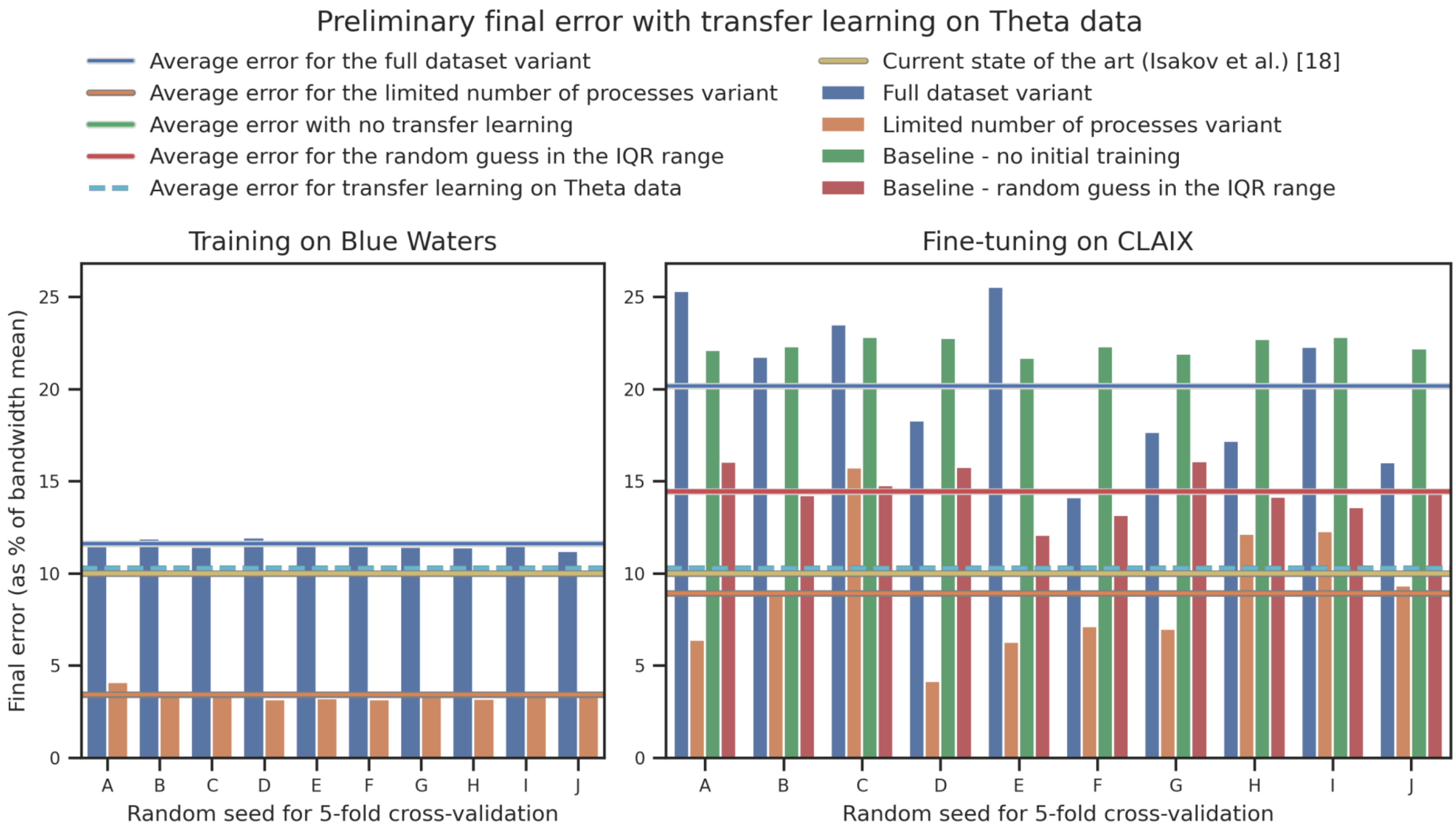


Comparison of results between the transfer learning stages (cont.)

Final errors across all stages and variants (as % of the mean bandwidth)

Variant	Initial training	Fine-tuning
Full dataset	11.6%	20.1%
Limited number of processes	**3.4%**	**8.92%**
Random guess in the IQR	95.9%	14.4%
No initial training	-	22.4%
Current state of the art (Isakov et al.) [18]	10%	10%

Preliminary results using data from ALCF Theta



What did the model learn?

- Explainable AI lets us “take a look into the black box”
- Idea: Attribute importance to the features

- Multiple approaches available:
  - Integrated Gradients [4] (with NoiseTunnel [5])
  - DeepLift [6]
  - Feature Ablation [7]
  - Shapley Value Sampling [8, 9]
  - Guided Backpropagation [10]
  - Feature Permutation [11]
  - InputXGrad [12]
  - Saliency [13]

- Use **all the approaches** above to cross-compare the attributions

Top 10 most important features

$$MiB/s = \left(\frac{\sum_{rank=0}^{n-1} (bytes_r + \boxed{bytes_w})}{\boxed{\max_{rank=0}^{n-1} (t_{md} + t_r + t_w)}} \right)$$

- **Times:**
  - POSIX_F_READ_TIME
  - POSIX_F_META_TIME
  - POSIX_TOTAL_TIME
  - POSIX_F_MAX_READ_TIME
  - POSIX_F_WRITE_TIME
  - POSIX_F_SLOWEST_RANK_TIME
- **Sizes:**
  - POSIX_ACCESS2_ACCESS
  - POSIX_SLOWEST_RANK_BYTES
  - POSIX_MAX_READ_TIME_SIZE
  - POSIX_BYTES_WRITTEN
- **# of processes**

Conclusion

- The proposed workflow is shown to work in the proof-of-concept form
  - Cross-validation results are mostly stable for both clusters
  - Explainable AI identifies the features considered by Darshan crucial for the bandwidth as the most important ones for the model
  - The results imply the produced models can outperform the current state of the art
- Several aspects require additional work in the future
  - Verify the workflow using data from MPI-IO, HDF5, and other common I/O APIs
  - Try to target different filesystems (e.g., BeeGFS)
  - Increase the diversity of applications in the target dataset
  - Evaluate MAPE as the measurement of model accuracy
    - Has its own drawbacks → try to use it as a part of a two-component error function:
      - MAE for the low-bandwidth jobs
      - MAPE for the high-bandwidth jobs
  - Test the proposed workflow on the data from additional clusters
  - Experiment with alternative outlier removal techniques or the ways to increase the robustness of the models to outliers
  - Use additional FS information to make more informed predictions
  - Remove all the time-based features & try to predict the execution time for a job

Thank you for your attention!

More details:

https://publications.rwth-aachen.de/record/958007

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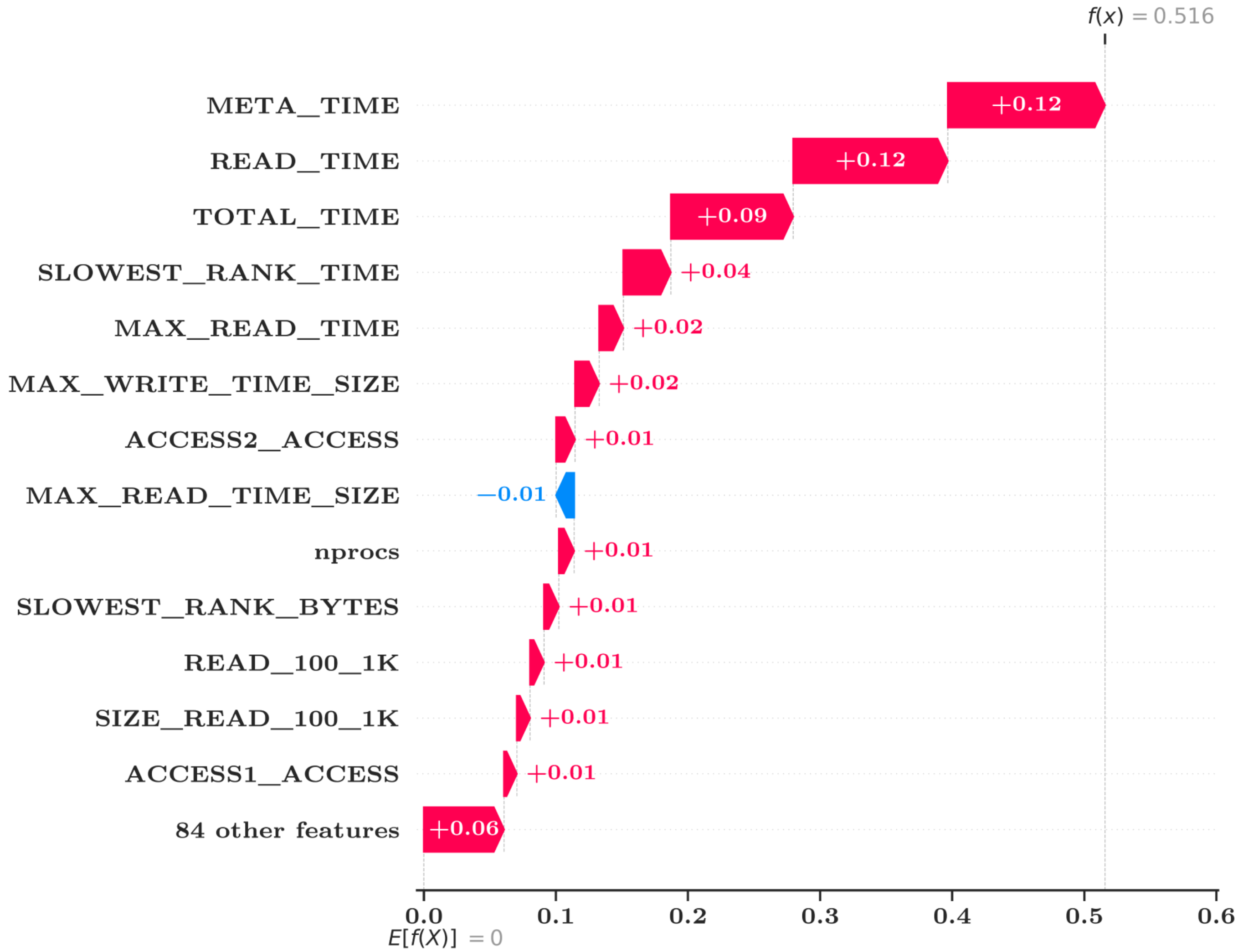
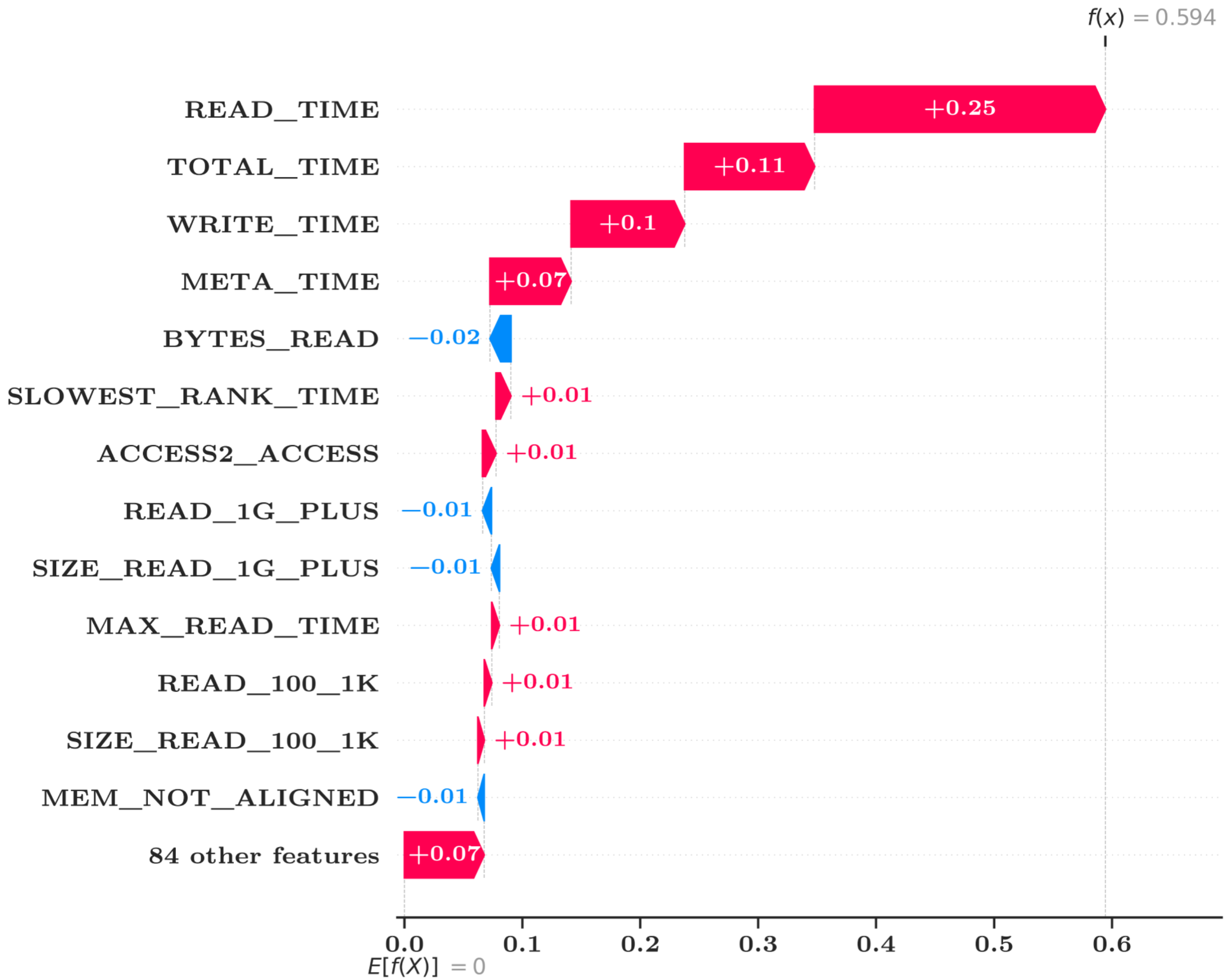
Appendix – Most important features (full dataset variant)



Appendix – Most important features (limited # of processes variant)



Appendix – Detailed model input

- POSIX_OPENS
- POSIX_FILENOS
- POSIX_DUPS
- POSIX_READS
- POSIX_WRITES
- POSIX_SEEKS
- POSIX_STATS
- POSIX_MMAPS
- POSIX_FSYNCS
- POSIX_FDSYNCS
- POSIX_RENAME_SOURCES
- POSIX_RENAME_TARGETS
- POSIX_RENAMED_FROM
- POSIX_MODE
- POSIX_BYTES_READ
- POSIX_BYTES_WRITTEN
- POSIX_MAX_BYTE_READ
- POSIX_MAX_BYTE_WRITTEN
- POSIX_CONSEC_READS
- POSIX_CONSEC_WRITES
- POSIX_SEQ_READS
- POSIX_SEQ_WRITES
- POSIX_RW_SWITCHES
- POSIX_MEM_NOT_ALIGNED
- POSIX_MEM_ALIGNMENT
- POSIX_FILE_NOT_ALIGNED
- POSIX_FILE_ALIGNMENT
- POSIX_MAX_READ_TIME_SIZE
- POSIX_MAX_WRITE_TIME_SIZE
- POSIX_SIZE_READ_0_100
- POSIX_SIZE_READ_100_1K
- POSIX_SIZE_READ_1K_10K
- POSIX_SIZE_READ_10K_100K
- POSIX_SIZE_READ_100K_1M
- POSIX_SIZE_READ_1M_4M
- POSIX_SIZE_READ_4M_10M
- POSIX_SIZE_READ_10M_100M
- POSIX_SIZE_READ_100M_1G
- POSIX_SIZE_READ_1G_PLUS
- POSIX_SIZE_WRITE_0_100
- POSIX_SIZE_WRITE_100_1K
- POSIX_SIZE_WRITE_1K_10K
- POSIX_SIZE_WRITE_10K_100K
- POSIX_SIZE_WRITE_100K_1M
- POSIX_SIZE_WRITE_1M_4M
- POSIX_SIZE_WRITE_4M_10M
- POSIX_SIZE_WRITE_10M_100M
- POSIX_SIZE_WRITE_100M_1G
- POSIX_SIZE_WRITE_1G_PLUS
- POSIX_STRIDE1_STRIDE
- POSIX_STRIDE2_STRIDE
- POSIX_STRIDE3_STRIDE
- POSIX_STRIDE4_STRIDE
- POSIX_STRIDE1_COUNT
- POSIX_STRIDE2_COUNT
- POSIX_STRIDE3_COUNT
- POSIX_STRIDE4_COUNT
- POSIX_ACCESS1_ACCESS
- POSIX_ACCESS2_ACCESS
- POSIX_ACCESS3_ACCESS
- POSIX_ACCESS4_ACCESS
- POSIX_ACCESS1_COUNT
- POSIX_ACCESS2_COUNT
- POSIX_ACCESS3_COUNT
- POSIX_ACCESS4_COUNT
- POSIX_FASTEST_RANK
- POSIX_FASTEST_RANK_BYTES
- POSIX_SLOWEST_RANK
- POSIX_SLOWEST_RANK_BYTES
- READ_0_100
- READ_100_1K
- READ_1K_10K
- READ_10K_100K
- READ_100K_1M
- READ_1M_4M
- READ_4M_10M
- READ_10M_100M
- READ_100M_1G
- READ_1G_PLUS
- WRITE_0_100
- WRITE_100_1K
- WRITE_1K_10K
- WRITE_10K_100K
- WRITE_100K_1M
- WRITE_1M_4M
- WRITE_4M_10M
- WRITE_10M_100M
- WRITE_100M_1G
- WRITE_1G_PLUS
- rank
- POSIX_F_READ_TIME
- POSIX_F_WRITE_TIME
- POSIX_F_META_TIME
- POSIX_TOTAL_TIME
- POSIX_F_MAX_READ_TIME
- POSIX_F_MAX_WRITE_TIME
- POSIX_F_FASTEST_RANK_TIME
- POSIX_F_SLOWEST_RANK_TIME