Scalable Neural Networks

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COM6012 Scalable Machine Learning

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Contents

Introduction

- This lecture will cover some topics at the interface of NNs and Spark
  - Will build up on your knowledge of NNs
- The intersection of deep learning and Spark is a very active field of research
- Several open source tools started developing in the last few years
  - Technical content is getting updated rapidly

Contents

Feedforward neural networks

- In this section, we will briefly review **feedforward neural networks** or **multilayer perceptrons**
- The MLP assumes that the input is a fixed-dimensional vector, say $\mathbf{x} \in \mathbb{R}^p$
- This data is referred to as "**unstructured data**": there are no assumptions about the form of the input
- Other types of neural networks assume that the input has variable size or shape
  - convolutional NN for variable-sized images
  - recurrent NN for variable-sized sequences
  - graph NN for variable-sized graphs

The Iris flower dataset

- The Iris flower dataset is a classic dataset used in pattern recognition
- It was introduced by the British statistician Ronald Fisher in a paper from 1936
- The dataset contains 150 instances
- Four input features: sepal length, sepal width, petal length, and petal width $\mathbf{x} \in \mathbb{R}^4$
- A categorical output, the species, which can take three values: Iris setosa, Iris virginica and Iris versicolor

Iris flowers

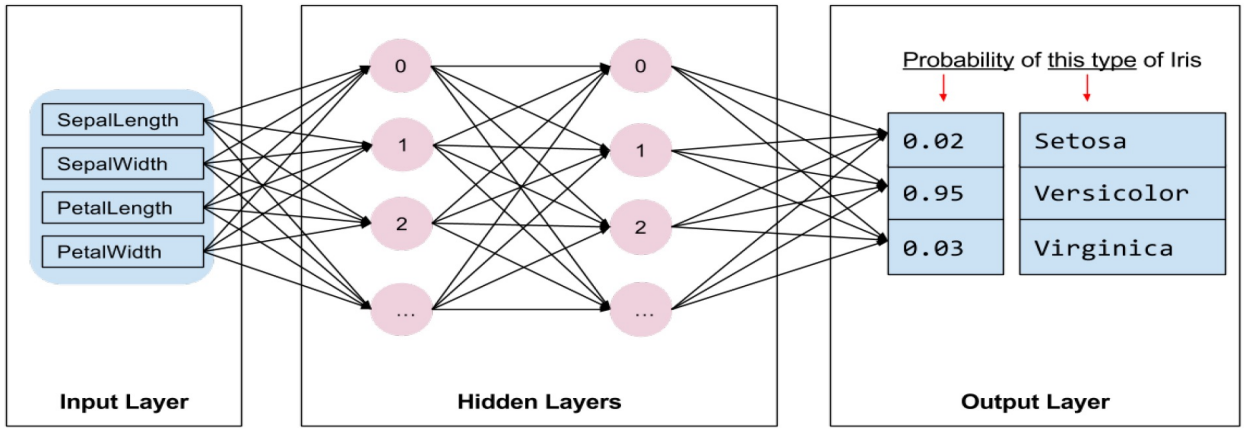
Iris versicolor

Iris setosa

Iris virginica

Source: https://en.wikipedia.org/wiki/Iris_flower_data_set

A 2-layer MLP applied to the Iris dataset



(a) A 2-layer MLP

$$p(y|\mathbf{x};\boldsymbol{\theta}) = \mathrm{Cat}(y|f_3(\mathbf{x};\boldsymbol{\theta}))$$
$$f_3(\mathbf{x};\boldsymbol{\theta}) = \mathcal{S}(\mathbf{W}_3 f_2(\mathbf{x};\boldsymbol{\theta}) + \mathbf{b}_3)$$
$$f_2(\mathbf{x};\boldsymbol{\theta}) = \varphi_2(\mathbf{W}_2 f_1(\mathbf{x};\boldsymbol{\theta}) + \mathbf{b}_2)$$
$$f_1(\mathbf{x};\boldsymbol{\theta}) = \varphi_1(\mathbf{W}_1 f_0(\mathbf{x};\boldsymbol{\theta}) + \mathbf{b}_1)$$
$$f_0(\mathbf{x};\boldsymbol{\theta}) = \mathbf{x}$$

(b) Mathematical model

$\boldsymbol{\theta} = (\boldsymbol{W_3}, \boldsymbol{b_3}, \boldsymbol{W_2}, \boldsymbol{b_2}, \boldsymbol{W_1}, \boldsymbol{b_1})$, $\mathcal{S}(\cdot)$ soft-max function, $Cat(\cdot)$ categoricaldistribution, φ_1, φ_2 activation functions

L-layer MLP

- An L-layer MLP is in general defined as a non-linear function

$$f(\mathbf{x}, \boldsymbol{\theta}) = f_L\left(f_{L-1}\left(\cdots\left(f_1(\mathbf{x})\right)\cdots\right)\right)$$

where $f_l(\mathbf{z}_{l-1}) = \varphi_l(\mathbf{W}_l\mathbf{z}_{l-1} + \mathbf{b}_l) = \mathbf{z}_l, \mathbf{z}_{l-1}$ are the hidden units at layer $l-1$ and $\varphi_l(\cdot)$ are the activation functions at layer l

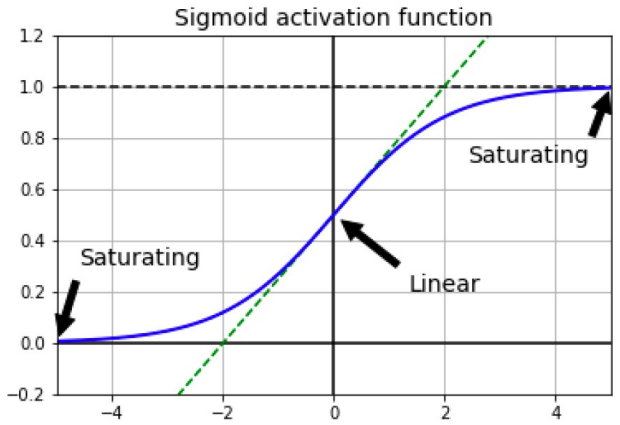
- In the expression above, $\boldsymbol{\theta} = [\boldsymbol{W}_L, \boldsymbol{b}_L, \cdots, \boldsymbol{W}_1, \boldsymbol{b}_1]$

- The activation functions $\varphi_l(\cdot)$ are non-linear, differentiable functions such that $\varphi_l: \mathbb{R} \to \mathbb{R}$

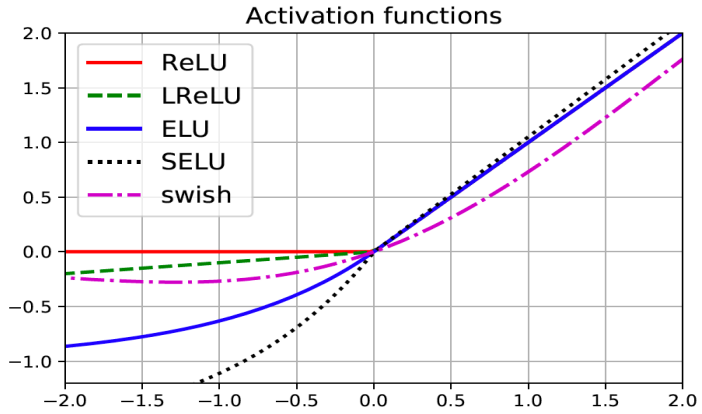
Activation functions φ_l

Name	Definition	Range
Sigmoid	$\sigma(a) = \frac{1}{1+e^{-a}}$	$[0, 1]$
Hyperbolic tangent	$\tanh(a) = 2\sigma(2a) - 1$	$[-1, 1]$
Softplus	$\sigma_+(a) = \log(1 + e^a)$	$[0, \infty]$
Rectified linear unit	$\mathrm{ReLU}(a) = \max(a, 0)$	$[0, \infty]$
Leaky ReLU	$\max(a, 0) + \alpha \min(a, 0)$	$[-\infty, \infty]$
Exponential linear unit	$\max(a, 0) + \min(\alpha(e^a - 1), 0)$	$[-\infty, \infty]$
Swish	$a\sigma(a)$	$[-\infty, \infty]$

(a) Mathematical form for different activation functions



(b) Sigmoid activation function



(c) Comparison of different activation functions

Backpropagation

- Remember that the backpropagation algorithm is used to compute the gradient of the loss function wrt the parameters of the NN (MLAI module)

- Once the gradient is computed, it is passed to a gradient-based optimization algorithm

Objective functions

- Given a dataset $\mathcal{D} = \{\mathbf{x}_n, \mathbf{y}_n\}_{n=1}^N$, the NN parameters are usually fit using maximum likelihood estimation

$$\text{NLL}(\mathcal{D}; \boldsymbol{\theta}) = -\log p(\mathcal{D}|\boldsymbol{\theta}) = -\sum_{n=1}^{N} \log p(\mathbf{y}_n|\mathbf{x}_n; \boldsymbol{\theta})$$

- Practical considerations when training deep models:
  - tuning the learning rate
  - vanishing gradient problem. Solutions: modify the architecture (residual connections), standardize the activations at each layer (batch normalization) and careful parameter initialization
  - exploding gradients. Addressed with gradient clipping

Contents

`MultilayerPerceptronClassifier` (I)

- Spark ML implements feed-forward neural networks through the `MultilayerPerceptronClassifier class`

- Nodes in the intermediate layers use the logistic sigmoid function

$$\varphi_l(z_i) = \frac{1}{1 + \exp(-z_i)}$$

- Nodes in the output layer use the softmax function

$$\mathcal{S}(z_k) = \frac{\exp(z_k)}{\sum_{c=1}^{K} \exp(z_c)}$$

where *K* is the number of classes corresponding to the same number of nodes in the output layer

`MultilayerPerceptronClassifier` (II)

- Spark ML uses backpropagation for learning the model
- L-BFGS is the default optimization routine
- The parameter `layers` specifies the number of layers and the number of nodes per layer, from input layer to output layer
- E.g. if `layers` = [780, 100, 10], this means a NN with 780 inputs, one hidden layer with 100 nodes and an output layer with 10 classes

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Beyond Spark ML

- Spark ML is not always the best solution for our machine learning needs
  - Predictions that require super low-latency (e.g. real-time, less than 10ms)
  - It does not have support for the algorithm we would like to use, e.g. deep learning
- In this cases, we can still use Spark, but not Spark ML
- There are different alternatives to use external models inside Spark ML
- For example, we can use Pandas UDFs (user-defined functions) for distributed inference of single-node models

Contents

Deep learning and Spark

- Three major ways to use deep learning in Spark
  - Inference
  - Featurization and transfer learning
  - Model training

Inference

- The simplest way to use deep learning is to use a pretrained model to make predictions in large datasets in parallel using Spark
- For example, the InceptionV3 model, a large neural network model for object recognition can be applied to our own collection of images
- In principle, one can simply use PySpark with a call to a framework like TensorFlow or Pytorch in a `map` function to get distributed inference
- In practice, there are further optimizations that can be made to make such a call efficient

Featurization and transfer learning

- We can also use an existing model as a *feature extractor* instead of taking its final output
- As you probably know by now, deep learning models tend to learn useful feature representations in their lower layers
- Low-level features learned in Imagenet can be used a starting point to learn new models in a different datase
- This method is called *transfer learning* and it is particularly useful when we do not have a large amount of training data for the new problem

Model training

- Spark can also be used to train a new deep learning model from scratch
- One can either train a *single* model over multiple executors communicating between them
- Or one can train *multiple* instances of similar models in parallel to try various model architectures and hyper-parameters

Contents

What are UDFs?

- Spark SQL has a lot of built-in functions that can be applied to dataframes
- Spark is flexible enough to allow users to define their own functions
- These are known as *user-defined-functions* (UDFs)
- A typical example in data analytics:
  - wrap a ML model within an UDF
  - query its predictions in Spark
  - there is no need to understand the internal behavior of the model SQL

PySpark UDFs before Spark 2.3

- Up until Spark 2.3, a permanent issue with PySpark UDFs was that they had lower performance compared with Scala UDFs

- The reason for this was that PySpark UDFs required data movement between JVM and Python, which was expensive

- For details, see Speeding up PySpark with Apache Arrow by Bryan Cutler

PySpark UDFs from Spark 2.3

- Pandas UDFs, introduced in Spark 2.3, addressed this issue by using Apache Arrow to transfer data and Pandas to work with the data
- Once the data is in Apache Arrow, there is no longer the need to serialize the data as it is already in a format consumable by the Python process
- Instead of operating on individual inputs row by row, now the operation is over Pandas Series or DataFrame
  - This is what is known as vectorized execution

A simple example of speed-up

```
from pyspark.sql.functions import rand
df = spark.range(1 << 22).toDF("id").withColumn("x", rand())
df.printSchema()
```

```
root
 |-- id: long (nullable = false)
 |-- x: double (nullable = false)
```

```
%time pdf = df.toPandas()
```

```
CPU times: user 10.6 s, sys: 714 ms, total: 11.3 s
Wall time: 16.1 s
```

```
spark.conf.set("spark.sql.execution.arrow.enabled", "true")
```

```
%time pdf = df.toPandas()
```

```
CPU times: user 102 ms, sys: 134 ms, total: 236 ms
Wall time: 1.04 s
```

```
pdf.describe()
```

	id	x
count	4.194304e+06	4.194304e+06

PySpark UDFs from Spark 3.0

- From Apache Spark 3.0 with Python 3.6+, the Pandas UDFs were split into two API categories: Pandas UDFs and Pandas Function APIs
- Pandas UDFs
  - From Spark 3.0, Pandas UDFs infer the Pandas UDFs type from *Python type hints* such as `pandas.Series` or `pandas.Dataframes`
  - Previously, users were required to manually define and specify each Pandas UDF type
  - Currently, the supported cases of Python type hints in Pandas UDFs are
    - Series to Series
    - Iterator of Series to Iterator of Series
    - Iterator of multiple series to Iterator of Series
    - Series to Scalar.
    - All of the above replacing Series with DataFrame

PySpark UDFs from Spark 3.0

- From Apache Spark 3.0 with Python 3.6+, the Pandas UDFs were split into two API categories: Pandas UDFs and Pandas Function APIs

- Pandas Function APIs
  - They allow to directly apply a local Python function to a PySpark Dataframe where both the input and output are Pandas instances
  - Currently, the supported Pandas Function APIs are
    - Grouped Map with `groupBy().applyInPandas()`
    - Map with `mapInPandas()`
    - Co-grouped Map with `groupBy().cogroup().applyInPandas()`

- This week's lab will contain example of using `mapInPandas()` for making inference with a NN

- This blog post by Databricks provides more details on Pandas UDFs and Pandas Function APIs in Apache Spark 3.0

Iterator support in Pandas UDFs

- A typical use case for Pandas UDFs is to load a machine learning or deep learning model to perform distributed inference
- If the model is large (typical deep learning models can be tens or hundreds of Mbs), then there is a high overhead to load the same model again and again for every batch in the same Python process
- Pandas UDFs accept iterators of `pandas.Series` or `pandas.DataFrame`
- The pseudocode looks something like

```
@pandas_udf(...)
def predict(iterator):
    model = ... # load model
    for features in iterator:
        yield model.predict(features)
```

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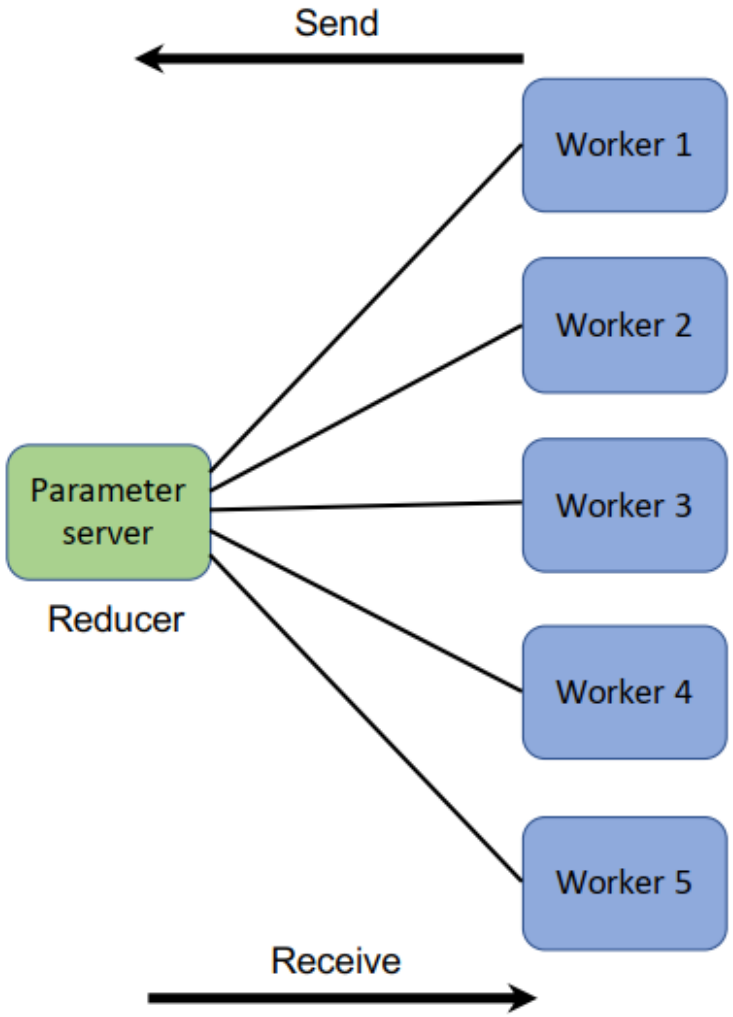
Horovod

- Horovod is an open-source software framework for distributed deep learning training using TensorFlow, Keras, PyTorch and MXNet
- It was developed by Uber
- Initial release was from August 2017 and the latest stable release is from May, 2020
- Details on the following slides are from the blog post Bringing HPC Techniques to Deep Learning by Andrew Gibiansky

The parameter server approach



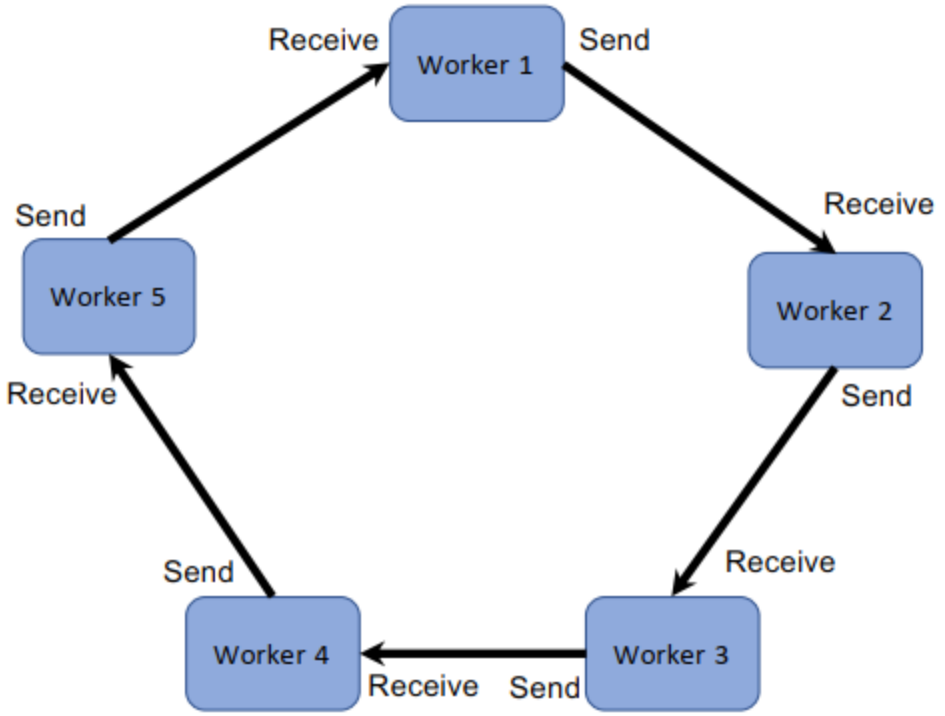
The parameter server approach

- Deep learning models have potentially millions of parameters
- For example, AlexNet has 60 millions of parameters. There are models today that have even billions of parameters – LLMs
- In the parameter server approach, each worker requires a complete copy of the neural network
- Sending the parameters of these NNs back and forward between the server and the workers creates a communication overhead that slow traininig
- The more workers in the system, the greater the communication cost

Ring reduce

- In contrast, ring reduce is an algorithm for which communication is constant
- If we only consider bandwidth as a factor in the communication cost, the ring allreduce is an optimal communication algorithm
- The workers in ring reduce are arranged in a logical ring

Ring allreduce

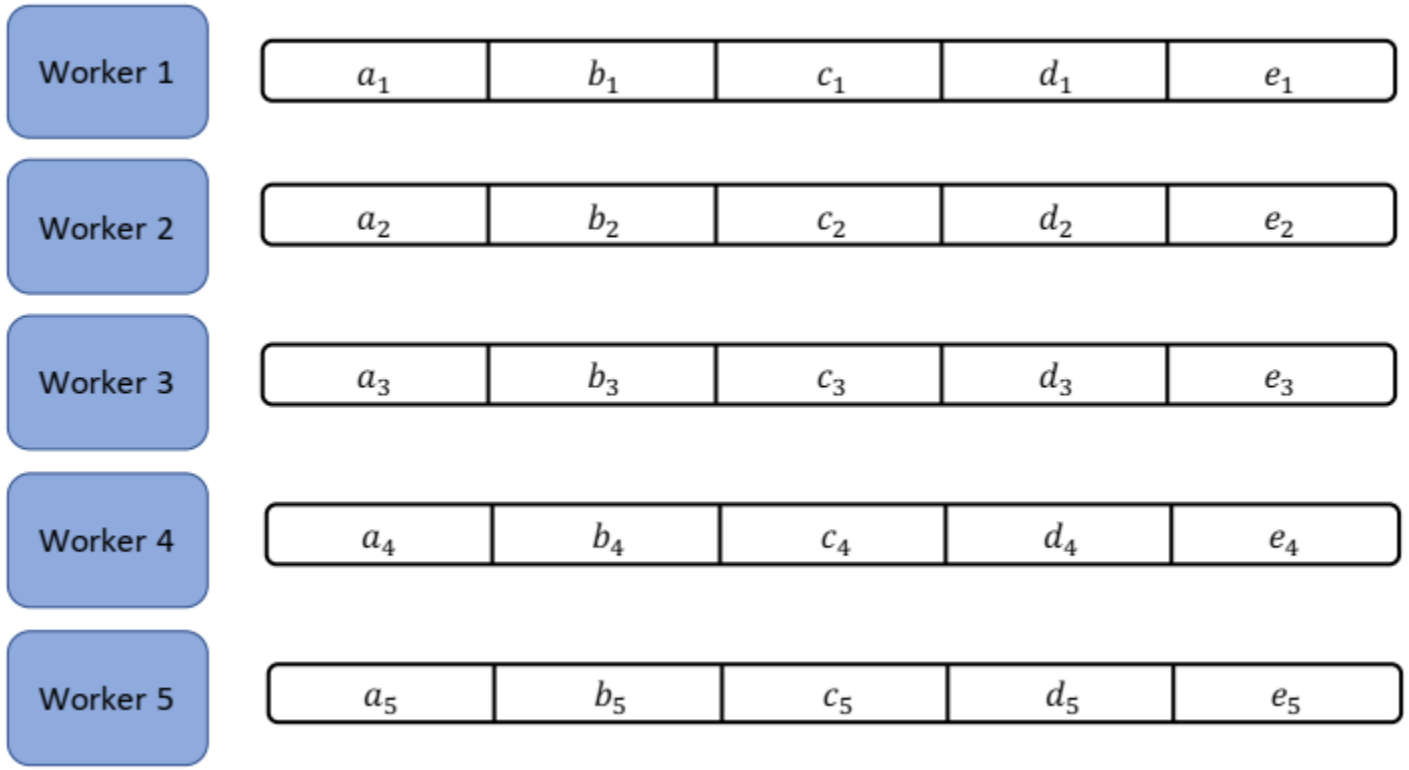


- Each worker has a right neighbour and a left neighbour
- Each worker sends data to its right neighbour and receives data from its left neighbour

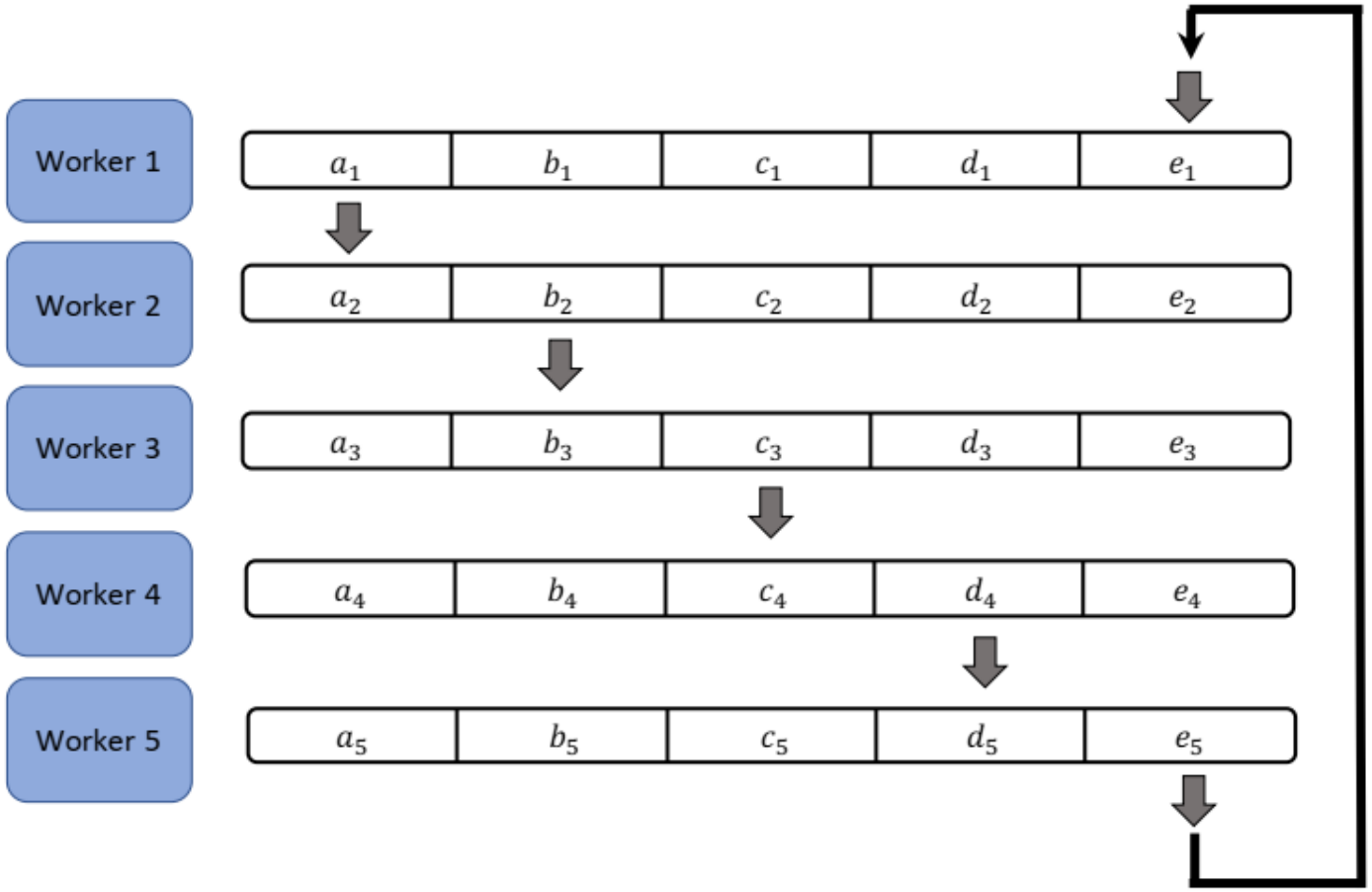
Ring allreduce: two-stages

- Ring all reduce is performed in two stages
- In the scatter-reduce stage, workers exchange data such that every worker ends up with a chunk of the final result
- In the allgather stage, the workers exchange those chunks such that eack worker ends up with the complete final result

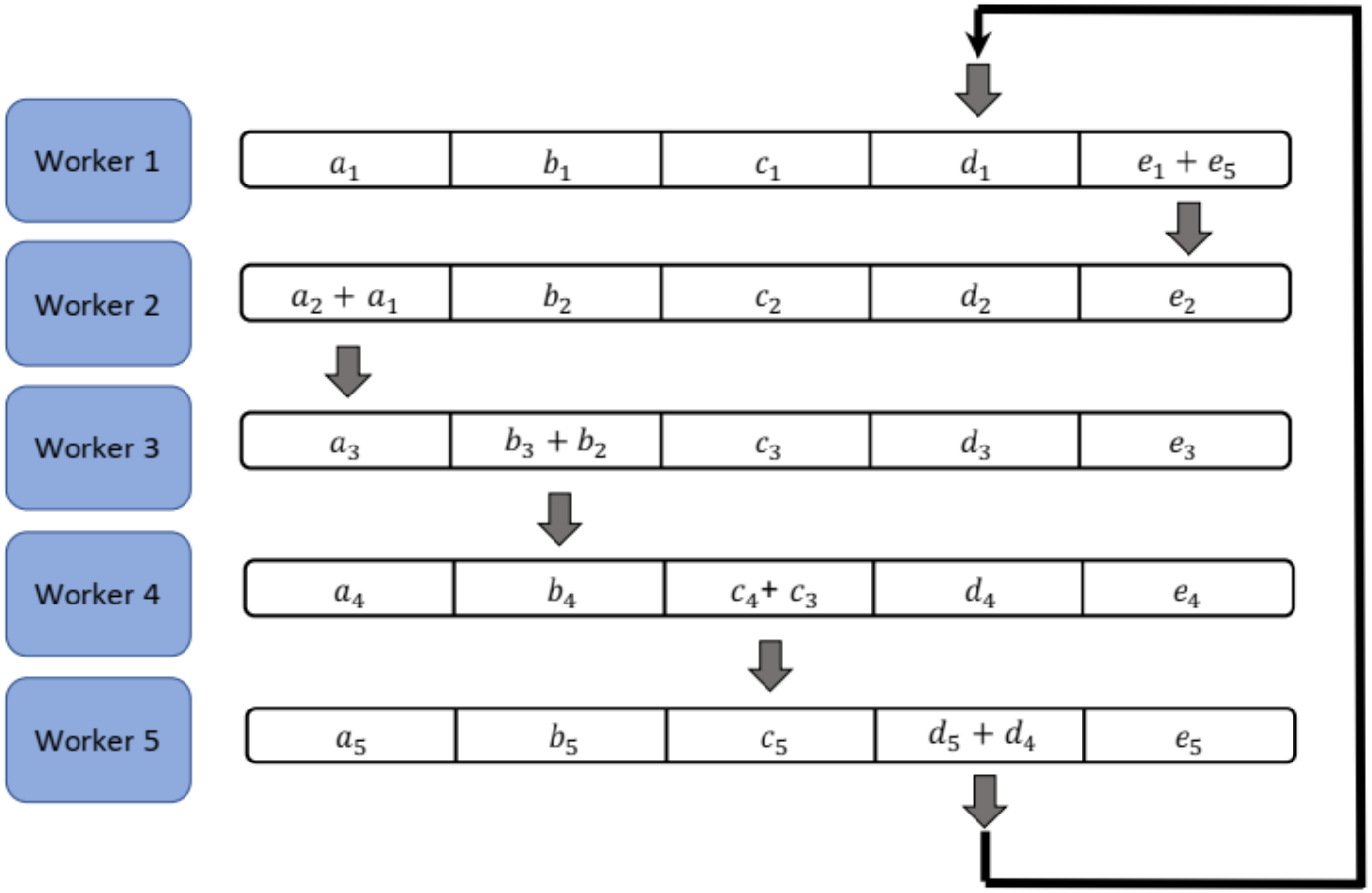
Summing arrays: scatter-reduce



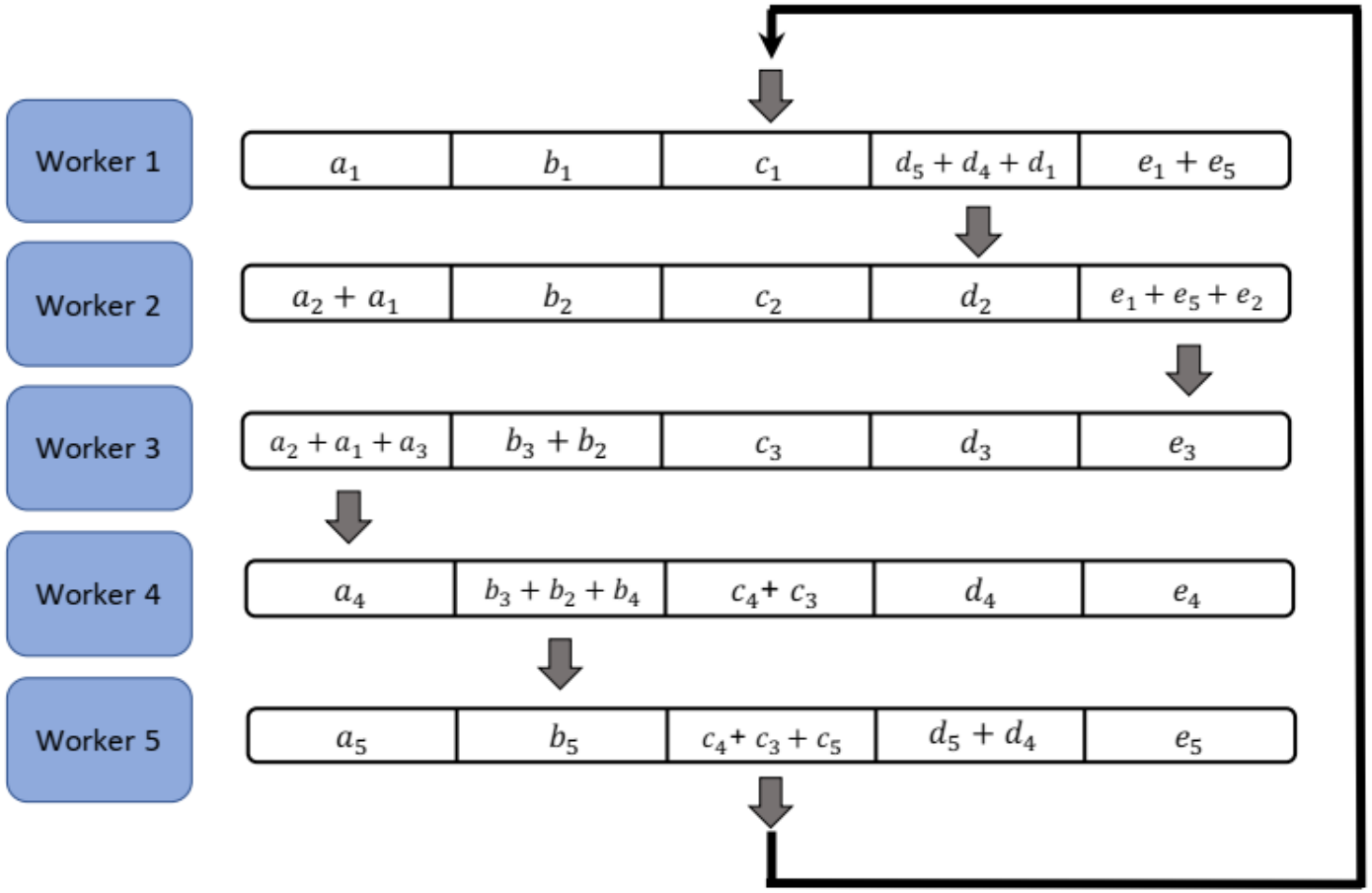
Summing arrays: scatter-reduce



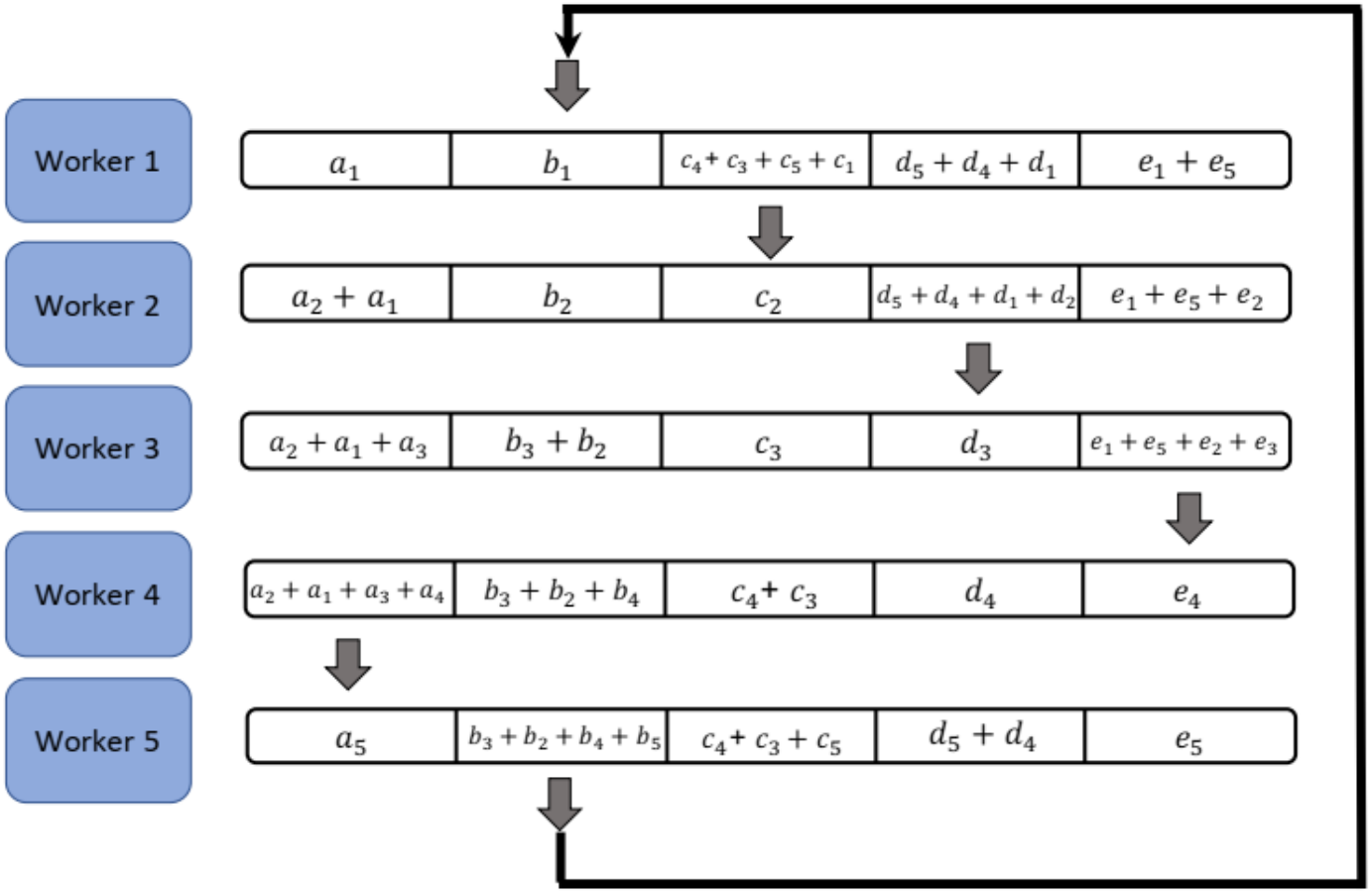
Summing arrays: scatter-reduce



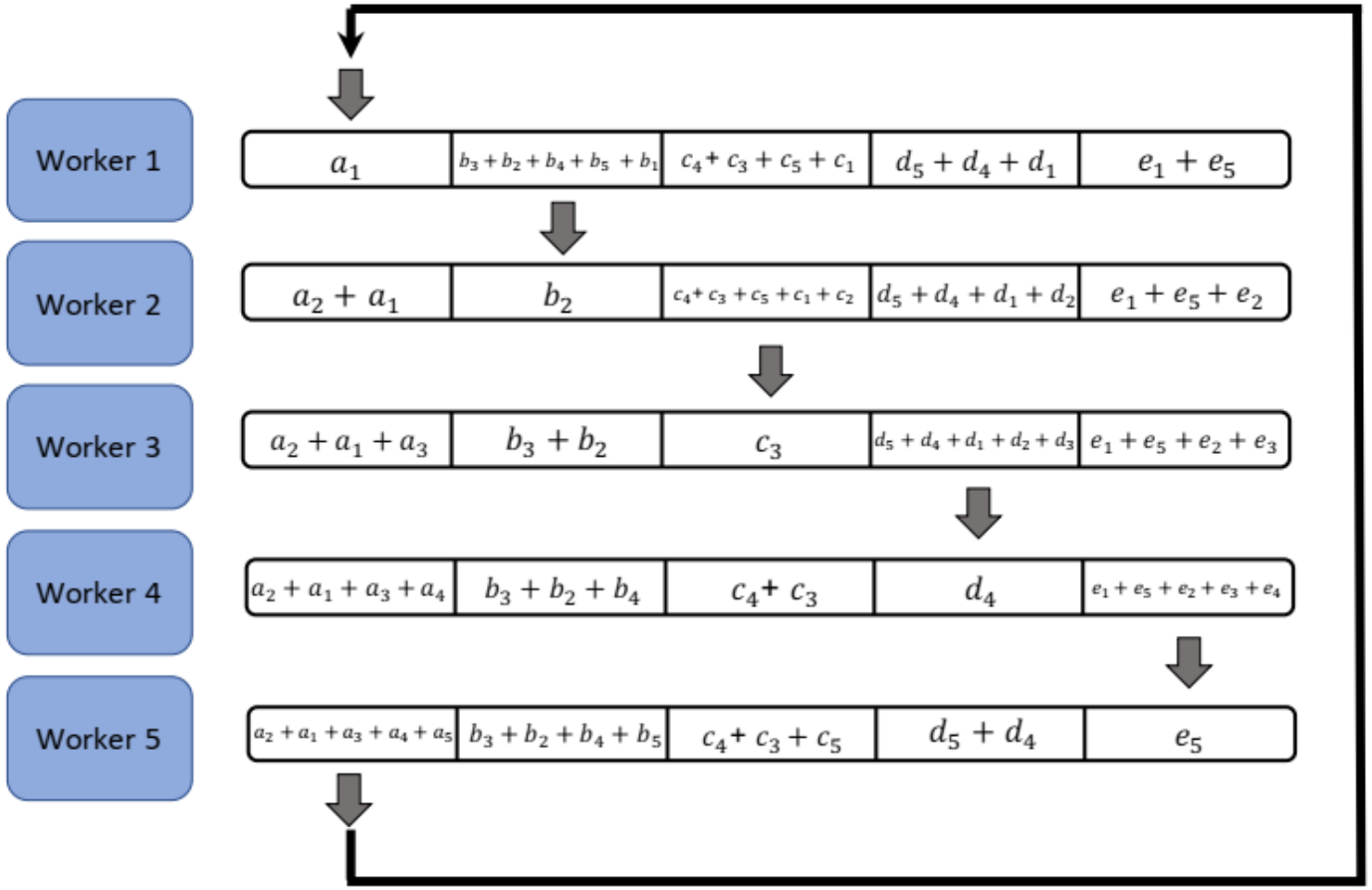
Summing arrays: scatter-reduce



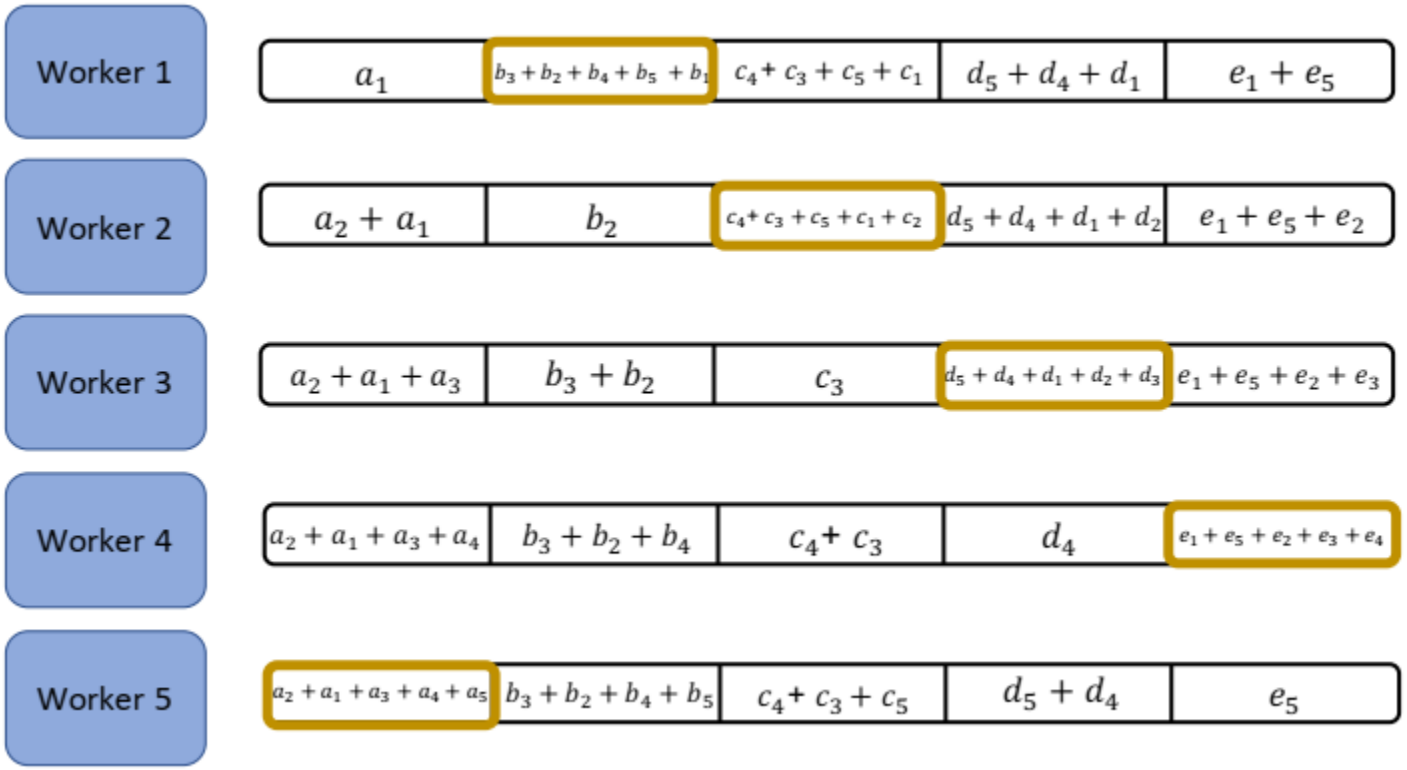
Summing arrays: scatter-reduce



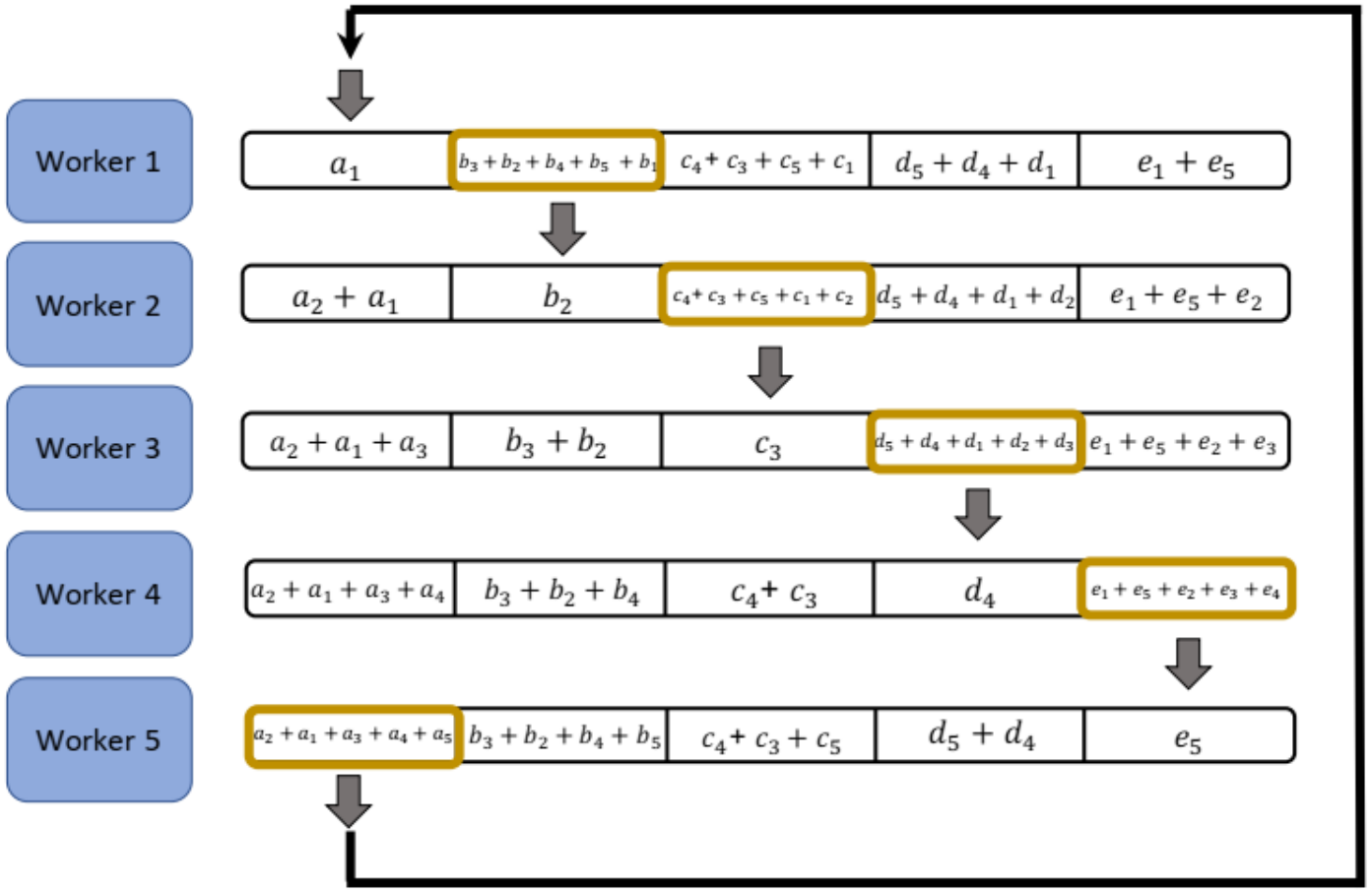
Summing arrays: scatter-reduce



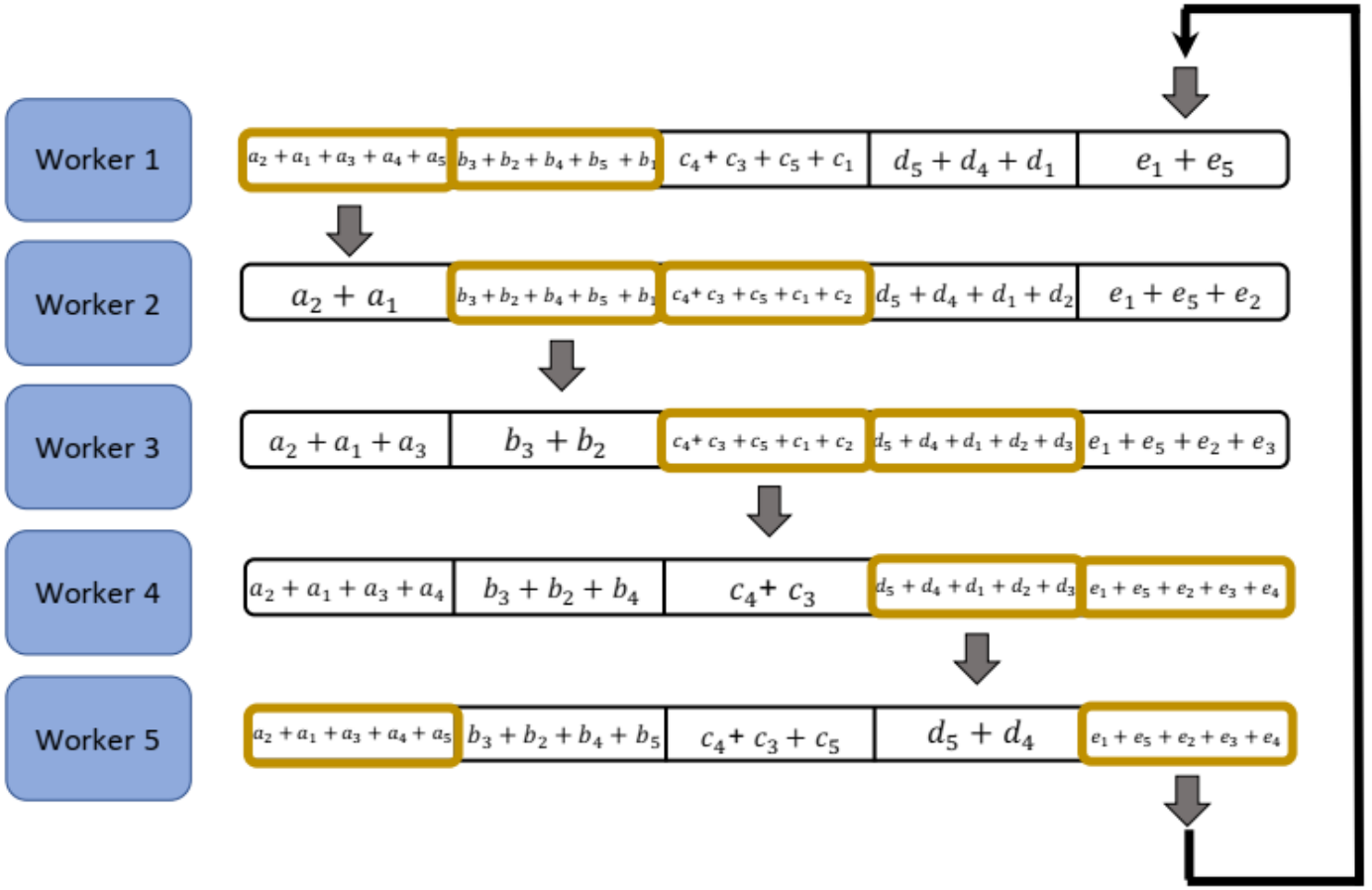
Summing arrays: scatter-reduce



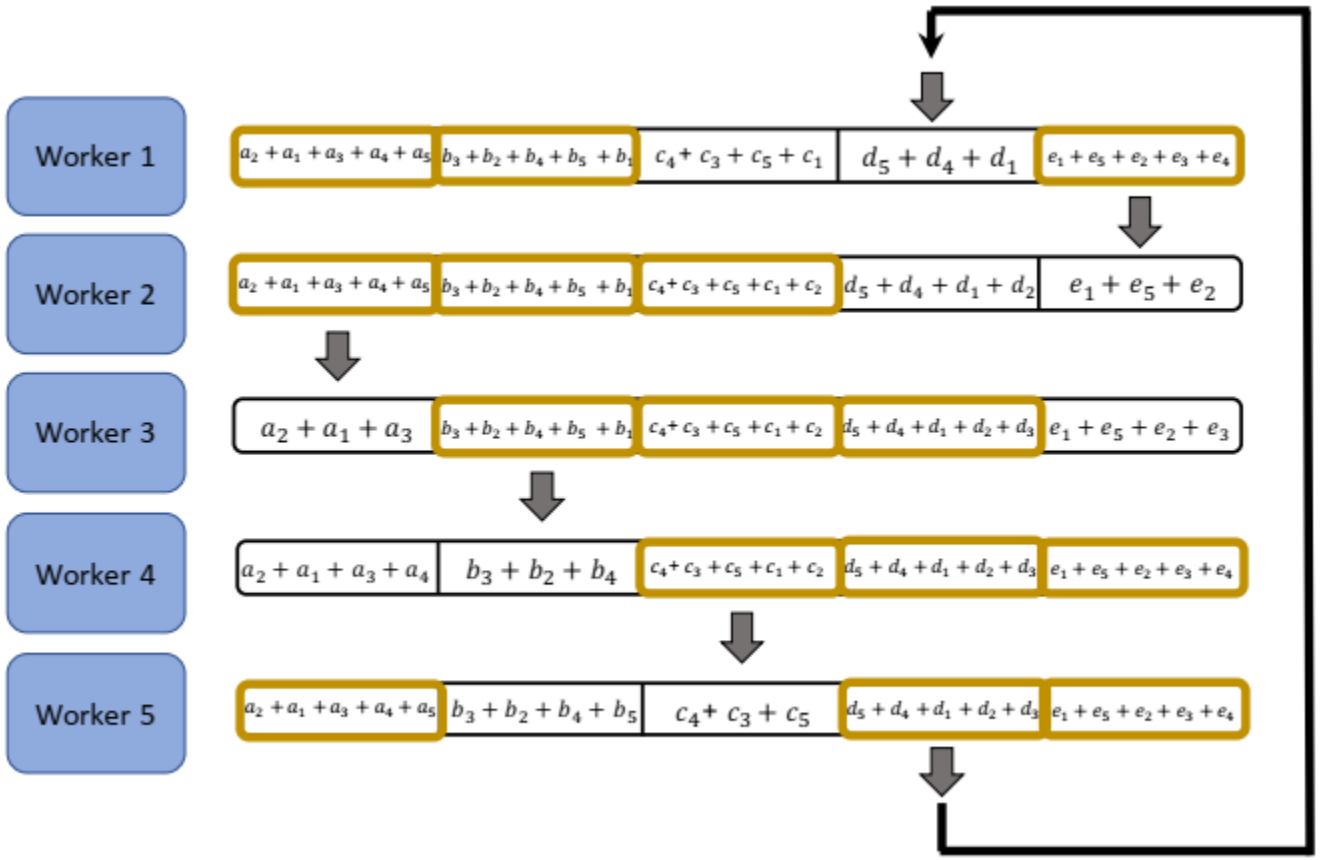
Summing arrays: allgather



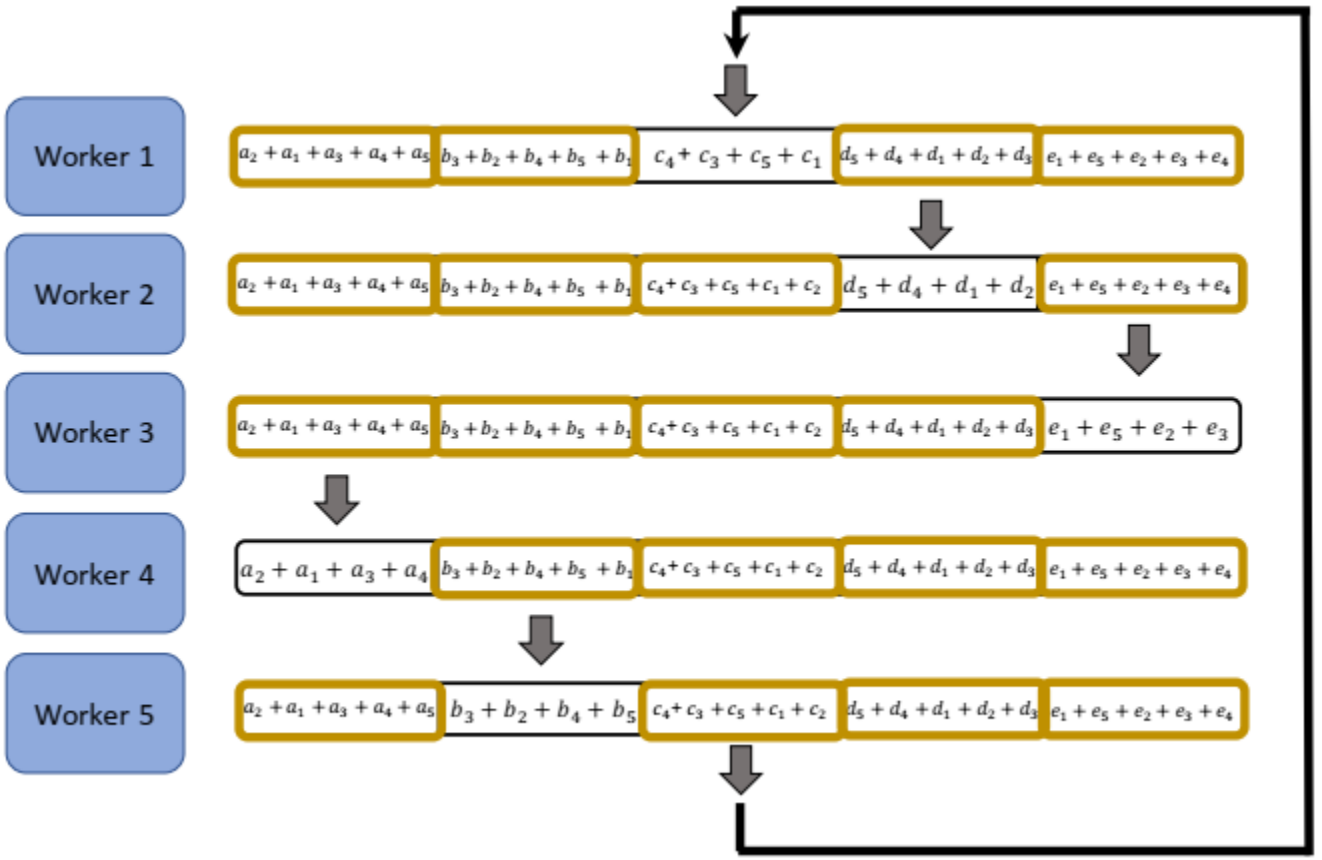
Summing arrays: allgather



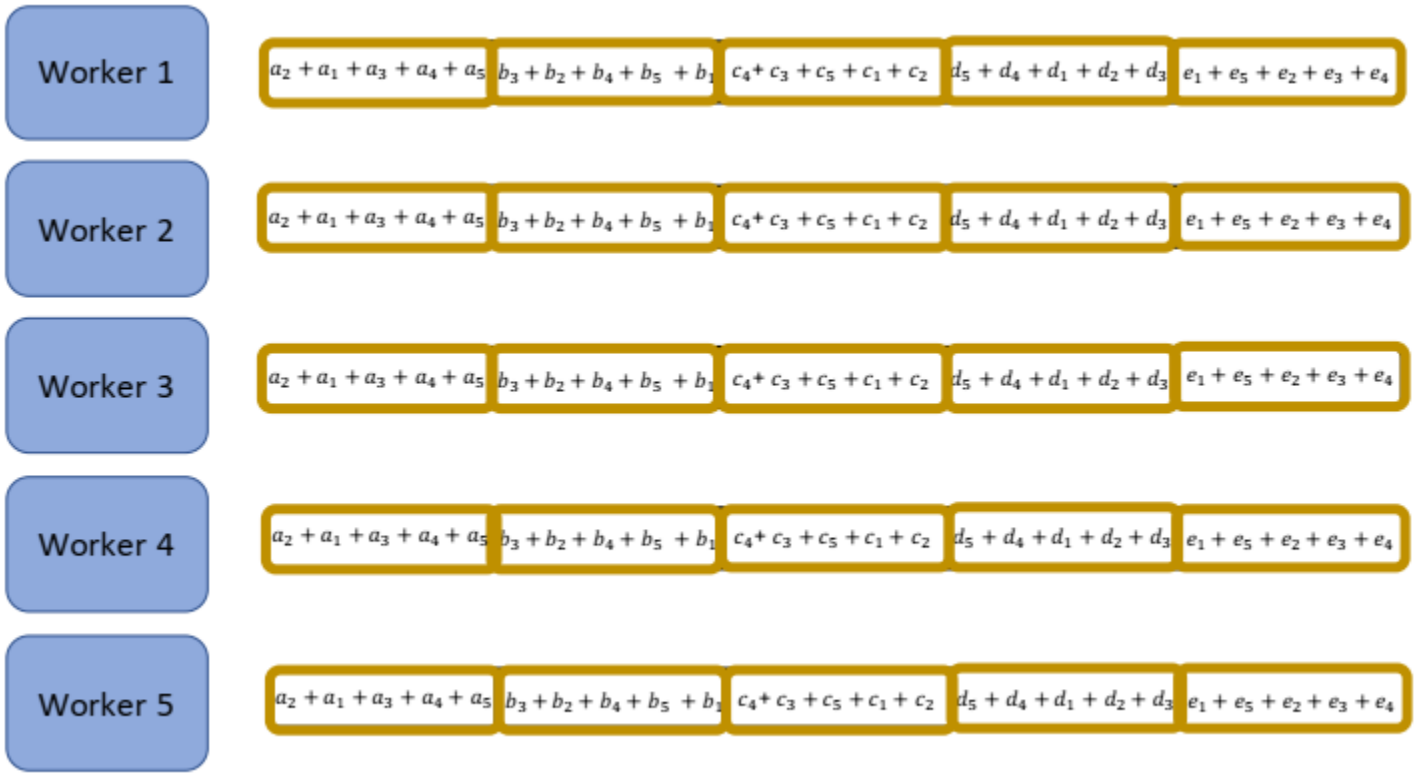
Summing arrays: allgather



Summing arrays: allgather



Summing arrays: allgather



Communication cost

- If there are *N* workers, each worker will send and receive values *N-1* times for scatter-reduce and *N-1* times for allgather
- Each time, the workers will send *K/N* values, where *K* is the total number of values in the array that are being summed across the different workers
- Then, the total amount of data transferred to and from every worker is

$$datatransferred = 2(N-1)\frac{K}{N}$$

which is independent of the number of workers

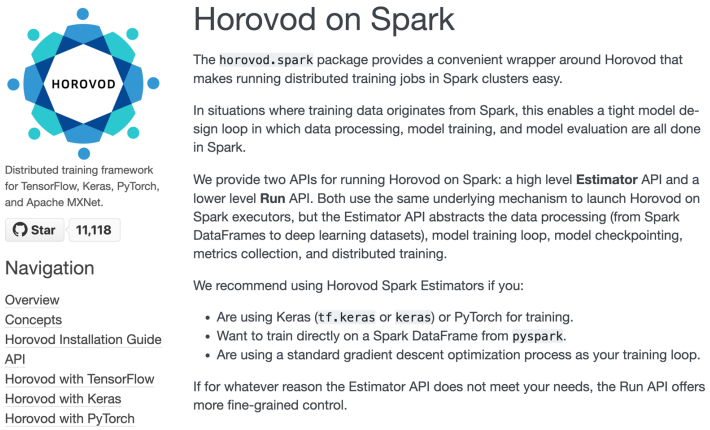
Origins of Horovod

- The idea of using ring allreduce to efficiently train deep learning models was introduced by a team at Baidu in early 2017
- Uber later adopted Baidu's draft implementation of the TensorFlow ring-allreduce algorithm and built upon it
- The resulting Python package was named Horovod, “named after a traditional Russian folk dance in which performers dance with linked arms in a circle”

Horovod dancing. Source: Wikimedia commons

Horovod on Spark

- Two APIs provided: a high level Estimator API and a lower level Run API
- The Estimator API is recommended if
  - training is done with Keras or PyTorch
  - you want to train directly on a Spark Dataframe from *pyspark*
  - you are using a standard gradient descent optimization process for training
- The Run API offers more fine-grained control



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Ray

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Ray provides a simple, universal API for building distributed applications.

Ray is packaged with the following libraries for accelerating machine learning workloads:

- Tune: Scalable Hyperparameter Tuning
- RLlib: Scalable Reinforcement Learning
- RaySGD: Distributed Training Wrappers
- Ray Serve: Scalable and Programmable Serving

There are also many community integrations with Ray, including Dask, MARS, Modin, Horovod, Hugging Face, Scikit-learn, and others. Check out the full list of Ray distributed libraries here.

Install Ray with: `pip install ray`. For nightly wheels, see the Installation page.

https://github.com/ray-project/ray

Analytics Zoo

Distributed TensorFlow, PyTorch, Keras and BigDL on Apache Spark & Ray

Analytics Zoo is an open source ***Big Data AI*** platform, and includes the following features for scaling end-to-end AI to distributed Big Data:

- Orca: seamlessly scale out TensorFlow and PyTorch for Big Data (using Spark & Ray)
- RayOnSpark: run Ray programs directly on Big Data clusters
- BigDL Extensions: high-level Spark ML pipeline and Keras-like APIs for BigDL
- Zouwu: scalable time series analysis using AutoML

For more information, you may read the docs.

https://github.com/intel-analytics/analytics-zoo

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Acknowledgement

Lecture slides were adapted from Dr Mauricio Alvarez, who contributed to this module from 2017 to 2022

Contents

References

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  - Probabilistic Machine Learning: An introduction by Kevin P Murphy, MIT Press, 2022 (https://probml.github.io/pml-book/book1.html)
  - Book: Spark: The Definitive Guide by Bill Chambers & Matei Zahaira, O'Reilly, 2018
  - Book: Learning Spark: Lightning-Fast Data Analytics by Jules Damji, Brooke Wenig, Tathagata & Denny Lee, O'Reilly, 2020
- Research paper:
  - Horovod: fast and easy distributed deep learning in TensorFlow by Alexander Sergeev and Mike Del Balso (https://arxiv.org/abs/1802.05799)
- Web resource:
  - Web resource: Spark Python API Documentation (https://spark.apache.org/docs/latest/api/python/reference/index.html)