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Sparse Linear Algebra in the Deep learning Framework

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Acknowledgements

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Lausanne, 12 Mars 2011

D. K.

Abstract

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Key words:

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Introduction

1 Sparse Data and Formats

Definition

Data are said sparse when it contains only a few non-null values. That kind of dataset are really common in Machine Learning application and can be an high influence on the computation.

The sparsity of a dataset is defined by :

$$sparsity = \frac{\# \text{ non-null values}}{\# \text{ values}} \quad (1.1)$$

Conversely when a dataset has only a few null values, the data are said dense. The density of the dataset is defined by the inverse of the sparsity:

$$density = \frac{1}{sparsity} \quad (1.2)$$

Using dense methods and data structure with sparse data could have a severe bad impact on the performance

The Advantages of Sparse Data

Sparsity is a very useful property in Machine Learning. Some algorithms can have fast optimization, fast evaluation of the model, statistical robustness or other computational advantages. A lot of machine learning application are using sparse dataset such as recommender system, natural language processing algorithm,

Sparse Data are very common in Machine Learning

In Machine Learning it's very common to deal with sparse dataset. We can encounter them in any kind of applications: Natural Language Processing, Retrieving Systems, Recommender Systems, etc.

Given the possible optimization that sparse dataset allows and the high number of people that could take advantages of it, it becomes important to add the support of sparse data in Nd4j.

A Real Case of Sparse Dataset

In 2008 Netflix launched a contest, the Netflix Grand Prize [net()], to improve their recommender system model and to increase the accuracy of predictions and published an sample dataset made with the ratings of anonymous Netflix customers. The dataset had more than 100 millions sampled ratings and it contained about $m = 480'186$ users and $m = 17'770$ movies [Koren(2009)]. If stored as a dense matrix, it would need to store $8'532'905'220$ values in memory. That corresponds to a sparsity $\cong \frac{100'000'000}{8'532'905'220} = 0.011719338$.

Storing more than 8 trillions 64-bit floating-point numbers needs more than 64 gigabyte of memory which quickly become unmanageable even for the world's fastest supercomputers.

Solution: Encode the data into a Sparse Format

To avoid the issue due to the high volume of storage needed, we must store the data into a sparse format. There are different kind of formats which each of them is more suitable to different aspects (Storage vs computation).

Formats

There are many methods for storing sparse data, each of them presents different advantages and disadvantages.

Matrices

Coordinates Format

It is the simplest method to encode a sparse array. The coordinates and the value of each non-zero entry are stored in arrays. Typically each element are encoded in a tuple (row, column, value)

Some implementation variations of the COO format exist. The elements can be sorted along a dimension, or it can have duplicate indexes.

$$A_{(M \times N)} = \begin{bmatrix} 0 & 2 & 0 \\ 0 & 0 & 3 \\ 1 & 0 & 4 \\ 0 & 0 & 0 \end{bmatrix} \rightarrow \begin{aligned} \text{Values}_{(1 \times NNZ)} &= [2 \quad 3 \quad 1 \quad 4] \\ \text{Rows}_{(1 \times NNZ)} &= [0 \quad 1 \quad 2 \quad 2] \\ \text{Columns}_{(1 \times NNZ)} &= [1 \quad 2 \quad 0 \quad 2] \end{aligned}$$

Figure 1.1: A matrix stored in COO format

This format provides an easy and fast way to retrieve a value and to insert a new non-zero element. It's also fast and simple to convert into a dense format.

But this format is not the most efficient regarding the memory consumption.

Compressed Row Format

The Compressed Row and the Compressed Column formats are the most general format to store a sparse array. They don't store any unnecessary element conversely to the COO format. But it requires more steps to access a element than the COO format.

Each non-zero element of a row are stored contiguously in the memory. Each row are also contiguously stored.

The format, described by the Intel MKL Sparse Library [mkl()], requires four arrays:

Values	All the nonzero values are store contiguously in an array. The array size is NNZ.
Column pointers	This array keeps the column position for each values.
Beginning of row pointers	Each pointer i points to the first element of the row i in the values array. The array size is the number of rows of the array.
End of row pointers	Each pointer i points to the first element in the values array that does not belong to the row i . The array size is the number of rows of the array.

Compressed Column Format

The Compressed Column Format is similar to CSR but it compresses columns instead of rows.

Given a matrix $N \times M$, the pointers arrays will have a size M .

$$A_{(N \times M)} = \begin{bmatrix} 0 & 2 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 4 & 0 \\ 0 & 0 & 2 & 1 \end{bmatrix} \rightarrow \begin{aligned} \text{Values}_{(1 \times NNZ)} &= [2 \quad 3 \quad 1 \quad 4 \quad 2 \quad 1] \\ \text{Columns}_{(1 \times NNZ)} &= [1 \quad 2 \quad 0 \quad 2 \quad 2 \quad 3] \\ \text{pointersB}_{(1 \times N)} &= [0 \quad 1 \quad 2 \quad 2 \quad 4] \\ \text{PointersE}_{(1 \times N)} &= [1 \quad 2 \quad 2 \quad 4 \quad 6] \end{aligned}$$

Figure 1.2: A matrix stored in CSR format

Tensors - Multi-dimensional arrays

A tensor is a multi-dimensional array. The order of the tensor is the dimensionality of the array needed to represent it. Matrices and vectors can be represented as tensors where the order is equals to 2 and 1 respectively.

This generalization allows a more generic implementation of a n-dimensional array in the Nd4j library.

Coordinates Format

The COO format can easily be extended to encode tensors by storing an array of indexes instead the row and column coordinates.

A array of order $K = 3$ with shape $N \times M \times P$ which has the following non-zero values :

value	indexes
1	0 1 0
2	1 1 2
3	1 2 0
4	2 0 1
5	2 2 0

can be encoded with one values array and one indexes array :

$$\begin{aligned} \text{Values}_{(1 \times NNZ)} &= [1, \quad 2, \quad 3, \quad 4, \quad 5] \\ \text{Indexes}_{(NNZ \times K)} &= [[0, 1, 0], \quad [1, 1, 2], \quad [1, 2, 0], \quad [2, 0, 1], \quad [2, 2, 0]] \end{aligned}$$

Figure 1.3: A tensor stored in COO format

2 The Deeplearning4j Library

Deeplearning4j is a open-source Deep Learning library for the JVM. It runs on distributed CPU's and GPU's.

→ TODO

Architecture of the library

The library is composed by several sub-libraries:

- Deeplearning4j** provides the tools to implement neural networks and build computation graphs
- Nd4j** is the mathematical back-end of Deeplearning4j. It provides the data structures for the n-dimensional arrays and allow Java to access the native libraries via JavaCPP and the Java Native Interface.
- Libnd4j** is the computing library that provides native operations on CPU and GPU. It's written in C++ and Cuda.
- Datavec** provides the operations for the data processing such that data ingestion, normalization and transformation into feature vectors.

The Importance of Nd4j in the Library

Nd4j is at the base of the Deeplearning4j library, it provides data storage, manipulations, and operations. It gives the atomic pieces needed to build more complex deep learning systems. Nd4j stands for N-Dimensional Arrays for Java and is basically a scientific computing library for the JVM. It features n-dimensional array object and the support of CPU and GPU via Cuda.

The APIs provided by the library are essentially wrappers for the different version of BLAS

(Basic Linear Algebra Subprogram).

BLAS is a specification that defines the low-level routines for linear algebra operations (for vectors and matrices). There exist several libraries implementing those subroutines in C or Fortran for dense or sparse formats. In Nd4j the BLAS subroutines can directly be called from Java thanks to JavaCPP, that internally uses the Java Native Interface (JNI) to call native routines from the JVM environment. This architecture allows the library to benefit from the advantages of the native side.

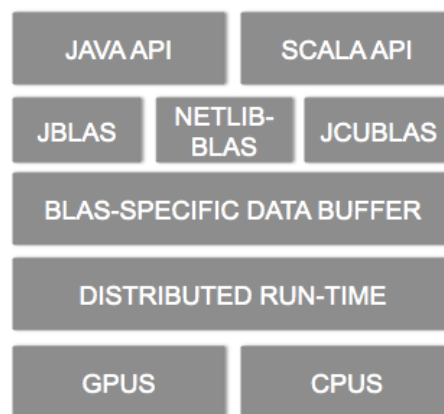


Figure 2.1: Nd4j architecture

Nd4j needs a Sparse Representation

Currently in Deeplearning4j, Sparse Data are treated as dense and use the dense operations of BLAS and Libnd4j to perform computations. With a new sparse representation we can gain in storage space and computation speed.

TODO -> develop

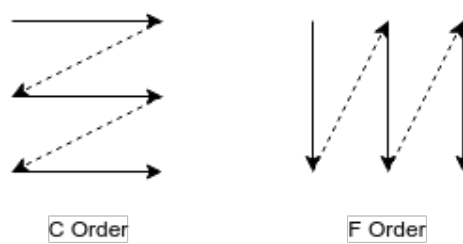
3 Structure of an Multi-dimensional Array

The new sparse array have to be compliant with the API and inter-operable with the current dense array implementation.

Storing an Array

A dense array is stored as a single contiguous block of memory, flatten in a one-dimensional array. Arrays are stored off-heap (outside the JVM environment). The reasons behind this design decision are numerous: better performance, better interoperability with BLAS libraries, and to avoid the disadvantages of the JVM such as the limited size of arrays due to the integer indexing (limited to $2^{31} - 1 \cong 2.14$ billion elements)

There are two methods to store a multi-dimensional array into a linear memory space: row-major order (C) or column-major order (Fortran). Figure 3.1 shows how a two-dimensional array is stored according to the order.



$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \end{bmatrix} \Rightarrow \begin{array}{l} C - Order = [a_{11} \ a_{12} \ a_{13} \ a_{21} \ a_{22} \ a_{23}] \\ F - Order = [a_{11} \ a_{21} \ a_{12} \ a_{22} \ a_{13} \ a_{23}] \end{array}$$

Figure 3.1: Comparison between C-order and F-order

The data are accessed via strides which define how to index over contiguous block of data. For each dimension it defines by how many values two consecutive elements are separated. In the case of matrix A defined in figure 3.1, the strides would be $(3, 1)$ in case of C-order and $(1, 3)$ in

Chapter 3. Structure of an Multi-dimensional Array

case of F-order. Strides (3, 1) means that each row is separated by 3 values and each column is separated by 1 value.

Data Buffer

The DataBuffer is a storage abstraction which provides optimal storage and retrieval depending on the backend. The data are stored off-heap through JavaCPP. It is basically a wrapper around a pointer and an indexer with utility methods to access and modify the data. The pointer points to the allocated memory space and the indexes provides an easy-to-use and efficient way to access a multi-dimensional memory space.

The implementation of the databuffer depends on the data type, because of the length needed to store a single value (int -> 32 bits, long -> 64bits, float -> 32bits, double -> 64bits)

Parameters of an Array

The information about the shape of the array are grouped in a DataBuffer object called ShapeInformation. It groups these following information:

Rank	The number of dimension of the array.
Shape	The shape of the array.
Strides	Provides information about the logical layout of the array for each dimension.
Offset	Provides the position of the first value of the data array that belongs to the array or view.
ElementWiseStride	Indicates how two contiguous elements are physically separated in memory.
Order	C or F order

Views

The data in memory can be shared by multiple NDArrays. An NDArrary can refer to a subset of another NDArrary. We say that such an array is a view of the original array. This is a powerful concept that avoid the unnecessary copy of the data which is a very expensive operation.

Since the memory space is shared, changes to one will impact the other ones. Figure ?? illustrates how a view shares its data with its original array.

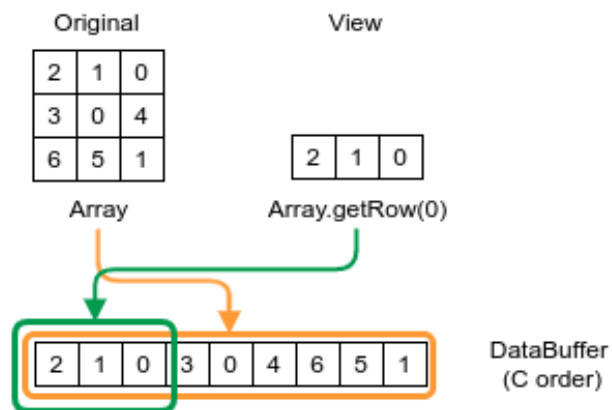


Figure 3.2: View shares memory with the original array

Indexes

NDArrays can be accessed through a combination indexes. ...

Operations

-> TODO briefly explain the different types of operation : Scalar Transform Accumulation
Index Accumulation Broadcast

4 Implementation

Hierarchy of Arrays

The API of an array is defined by an interface called `INDArray` which has a dense implementation for each backend: `NDArray` class for the CPU and `JCublasNDArray` class for the GPU. But since most of the operations and methods are shared between the two backends, they are implemented in an abstract class called `BaseNDArray`.

Adding sparse representations asked two questions:

1. What can be shared with the dense arrays ?
2. What can be between the different sparse arrays and what are format-specific ?

To answer those questions, we need to go a little bit deeper in the implementation.

... TODO

Finally we arrive at the conclusion that everything that can be shared between the formats can also be shared with the dense array. That's why the sparse implementations also extends from the `BaseNDArray` class. The implementations still need some format-specific methods which are overridden and implemented in the different `BaseSparseNDArray` classes.

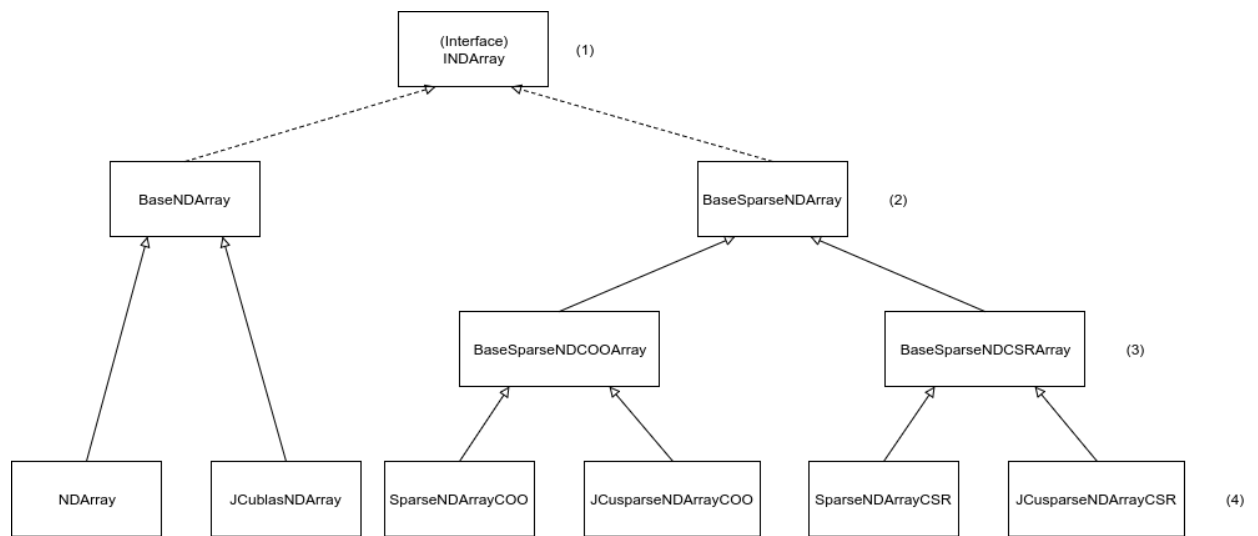


Figure 4.1: Arrays hierarchy in Nd4j

Limitations and Constraints

DataBuffers have a fixed length

CSR Matrices

Structure

Get or Put Data into this format

Limits with this format

COO Tensors

First implementation

More parameters are needed to define the tensors

All and Interval Indexes

Point Index

Specified Index

New Axis Index

Computations of the the Parameters

Computation of the Sparse Offsets

Computation of the Flags

Computation of the Hidden Dimensions

Sparse Indexes Translation

..

5 Operations

Backends

BLAS

Level 1 in CSR Matrix

Level 1 in COO Tensor

Libnd4j

..

6 Results

..

1

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7 Conclusion

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A An appendix

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