Owl: A General-Purpose Numerical Library in OCaml

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ABSTRACT
Owl is a new numerical library developed in the OCaml language. It focuses on providing a comprehensive set of high-level numerical functions so that developers can quickly build up data analytical applications. In this abstract, we will present Owl’s design, core components, and its key functionality.

1. INTRODUCTION
Thanks to the recent advances in machine learning and deep neural networks, there is a huge demand on various numerical tools and libraries in order to facilitate both academic researchers and industrial developers to fast prototype and test their new ideas, then develop and deploy analytical applications at large scale.

Python has been one popular choice among developers for fast prototyping analytical applications, one important reason is because Scipy \[6\] and Numpy \[2\] two libraries, tightly integrated with other advanced functionality such as plotting, offer a powerful environment which let developers write very concise code to finish complicated numerical tasks. As a result, even for the frameworks which were not originally developed in Python (such as Caffe and Tensorflow \[8\]), they often provide Python bindings to take advantage of the existing numerical infrastructure in Numpy and Scipy.

On the other hand, the libraries for supporting basic scientific computing in OCaml is rather fragmented. There have been some initial efforts (e.g., Lacaml, Oml, Pareto, and etc.), but they are either too low-level or are overly focused on a specific problem domain, hence developers often have to write a significant amount of boilerplate code just to finish some rather trivial numerical tasks. As we can see, there is a severe lack of a general purpose numerical library in OCaml. We believe OCaml per se is a good candidate for developing such a general purpose numerical library for two important reasons: 1) we can write functional code as concise as that in Python; 2) OCaml code often has much superior performance comparing to dynamic languages such as Python and Julia. In the following, we will introduce Owl\[1\] a new general purpose numerical library developed in OCaml. Owl can be easily installed with OPAM by executing "opam install owl".

2. CORE COMPONENT - NDARRAY
N-dimensional array and matrix are the building blocks of Owl library, their functionality are implemented in Ndarray and Matrix modules respectively. Matrix is a special case of n-dimensional array, and in fact many functions in Matrix module calls the functions in Ndarray directly.

For n-dimensional array and matrix, Owl supports both dense and sparse data structures. The dense data structure is built atop of OCaml’s native Bigarray module hence it can be easily interfaced with other libraries like BLAS and LAPACK. Owl also supports both single and double precisions for both real and complex number. Therefore, Owl essentially has covered all the necessary number types in most common scientific computations. The functions in Ndarray and Matrix modules can be divided into following three groups.

1) The first group contains the vectorised mathematical functions such as \(\sin\), \(\cos\), \(\text{relu}\), and etc. This group of functions are mostly implemented in C code to achieve the best performance.

2) The second group contains the high-level functionality to manipulate arrays and matrices, e.g., \(\text{ slicing}\), \(\text{ tile}\), \(\text{ repeat}\), \(\text{ padding}\), and etc.

3) The third group contains the linear algebra functions specifically for matrices. Almost all the linear algebra functions in Owl call directly the corresponding functions in BLAS and LAPACK.

Aforementioned three groups of functions together provide a strong support for developing high-level numerical functions. Especially the first two groups turn out to be extremely useful for writing machine learning and deep neural network applications.

3. OPERATORS FOR INTEROPERATION
OCaml does not support operator overloading at the moment which poses a big challenge when designing the operators in Owl. On one hand, it is desirable to use a set of unified and consistent operators so that we can

\[1\]https://github.com/ryanrhymes/owl
Algorithm 1 Build a Feedforward neural network

1: let network = input [] 784 []
2: |> linear 300 act_typ:Activation.Tanh
3: |> linear 100 act_typ:Activation.Softmax
4: in train network x y

write concise code for mathematical functions. On the other hand, we might lose some capability for static type checking since different number types are wrapped into the same type using different type constructors.

We have been leaning more towards readability and convenience when designing Owl’s operators. However, this does not necessarily mean we have to sacrifice the static type checking and performance in the library. The operators which allow interoperation on different number types are implemented in a specific module called Ext. Each operator in Ext corresponds to one specific function implemented in Owl. It means we can always choose to call the function directly instead of using operators for performance and type checking concerns. Operators are not meant to replace those functions, which leaves us to decide how and when to use them. By the time of writing, Owl has implemented over 20 common operators such as +, -, *, /, >, <, >, %, and etc.

4. ALGORITHMIC DIFFERENTIATION

Atop of the core components, we have developed several modules to extend Owl’s numerical capability. E.g., Maths module includes many basic and advanced mathematical functions, whilst Stats module provides various statistical functions such as random number generators, hypothesis tests, and so on. The most important extended module is Algodiff, which implements the algorithmic differentiation functionality [4,5].

The Algodiff module essentially bridges the gap between low-level numerical functions and high-level advanced analytical tasks such as optimisation, regression, and machine learning. Owl’s algorithmic differentiation module implements both forward and backward mode and supports arbitrarily higher-order derivatives. Because Algodiff.Generic is implemented as a functor that takes aforementioned Matrix and Ndarry module as inputs, it supports both single and double precisions.

With such capability, developing advanced data analytical applications become trivial. E.g., we can write up the core back-propagation algorithm in neural network from scratch in just 13 lines of OCaml code. Even better, we have already included a specific module in Owl for developing applications of deep neural networks. The code snippet (1) implements a simple feedforward neural network which can be used to recognise handwritten digits. Moreover, we can also use Owl to build more complicated neural networks with graph topology such as Google’s Inception network.

Owl is able to visualise the computation graph used in the algorithmic differentiation. The computation graph contains the detailed information of operators and operands, including the type information and shape of the data. The Fig. ?? demonstrates the computation graphs from a simple math function let f x y = Maths.(x * sin (x + x) + ( F 1. * sqrt x) / F 7.) * (relu y) |> sum, whilst Fig ?? shows the one from a VGG-like neural network.

Figure 1: The computation graph used in differentiating a simple math function in reverse mode.

5. PRELIMINARY COMPARISON

Performance is the key in many numerical applications, we have performed one preliminary evaluation of Owl lately, and the initial results appear promising.

We use Owl (version 0.2.0) in the evaluation and compare to Numpy (version 1.8.0rc1) and Julia (version 0.5.0) [1]. All evaluations are done on the same MacBook Air (1.6GHz Intel Core i5, 8GB memory).

We evaluate eight vectorised math functions and two iteration operations: +, *, map, and etc. Each operation is performed 10 times and the average time is reported. All the ndarrays used in the evaluation are of the shape 10 x 1000 x 10000, Float64 type, therefore 100 million double precision float numbers in each ndarray. The table below presents the results, i.e., the average time (in seconds) needed to finish the tested operations. We can see Owl achieves the best performance in these tests, but we acknowledge that Julia
Table 1: Performance comparison between Owl and other numerical libraries

|       | Owl  | Numpy | Julia |
|-------|------|-------|-------|
| empty | 0.0000 | 0.0000 | 0.0000 |
| create | 0.4051 | 0.4155 | 0.4874 |
| x + y  | 0.5402 | 0.5698 | 0.7514 |
| x * y  | 0.5330 | 0.5963 | 0.8649 |
| x + 2  | 0.4791 | 0.5246 | 0.6299 |
| x < y  | 0.1529 | 0.2209 | 0.6248 |
| abs x  | 0.4956 | 0.5186 | 0.5932 |
| map x  | 2.2181 | 51.4562 | 2.2582 |
| iter x | 0.4429 | 37.6902 | 6.4385 |

can be faster in some cases. In general, Owl and Julia possess similar performance.

6. DISTRIBUTED AND PARALLEL COMPUTING USING ACTOR SUBSYSTEM

The design on distributed and parallel computing module essentially differentiates Owl from other mainstream numerical libraries. For most libraries, the capability of distributed and parallel computing is often implemented as a third-party library, and the users have to deal with low-level message passing interfaces. However, Owl achieves such capability through its Actor subsystem.

The Actor subsystem implements three computation engines to handle both data-parallel and model-parallel computational jobs, as the following list shows.

1. **Map-Reduce**: implements APIs like `map`, `reduce`, `collect`, and etc. The engine is for data-parallel computational jobs.

2. **Parameter Server**: implements APIs like `register`, `push`, `pull`, and etc. The engine is for model-parallel jobs.

3. **Peer-to-Peer**: very similar to Parameter Server engine but without centralised server, each node in the system can serve part of the model.

Owl’s numerical functionality is "glued" with the Actor’s distribution functionality using a well-defined function to achieve distributed analytics. The users do not need to deal with low-level message passing since this is already implemented in the engines. The users only need to focus on the high-level application logic by selecting the proper engine to use.

Actor’s engine can be used to distributed and parallelise both low-level and high-level data structures. E.g., the following code implements a distributed Ndarray by combining Owl’s native Ndarray module and Actor’s map-reduce engine.
module M1 = Owl_parallel.Make (Dense.Ndarray.S) (Actor.Mapre)

The following code on the other hand implements a neural network module for distributed training by combining Owl’s Neural module and Actor’s Parameter Server engine.

module M2 = Owl_neural_parallel.Make (Neural.S.Graph) (Actor.Param)

7. CONCLUSION

In this abstract, we presented Owl - a new general purpose OCaml numerical library for developing advanced analytical applications. We introduced Owl’s design principles, as well as its core components, key functionality, advanced algorithmic differentiation. We also provided a small neural network example to show how to take advantage of Owl to fast prototype new ideas. Our preliminary evaluation has shown that Owl has superior performance comparing to other popular numerical libraries, meanwhile it lets developers to write concise code to finish complicated numerical tasks.

Future development will focus on the following aspects:

1. Owl’s core modules are distributed under MIT license except a couple depending on GSL. We will remove such dependency in future.

2. We will introduce Zoo system to facilitate code sharing and scripting in Owl.

3. We will interface to OpenCL to support offloading computation to GPU and FPGA.

8. REFERENCES

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