

KARLSRUHER INSTITUT FÜR TECHNOLOGIE

IMPLEMENTATION DOCUMENT (FSD)

Numerical Linear Algebra meets Machine Learning

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Contents

1	Introduction	3
2	Changes on the Design	3
3	The Requirements	3
3.1	Following Requirements are accomplished	3
3.2	Following Requirements were accomplished as far as possible	4
3.3	Following Requirements were not accomplished	5
4	Unittests	5
4.1	Controller	5
4.1.1	test_command_parser	5
4.1.2	test_controller	6
4.2	model	6
4.2.1	test collector	6
4.3	shared	6
4.3.1	test configurations	6
4.4	view	7
4.4.1	test cli output service	7
5	Delays and Problems	7
5.1	Labeling module	7
5.2	MVC	8
5.3	Training module	8
6	Lessons learned	8
7	Statistics	8
7.1	Work Splitting	8
8	Development model	9
8.1	Communication in the team	9
8.2	Git	9
9	Glossary	10

1 Introduction

Goal was the delivery of a consistent software stack that allows for employing neural networks for the linear system. The ecosystem should allow to train a neural network on selecting a suitable iterative solver depending on the linear system characteristics.

Since we were dealing with a big Python project for the first time and we've never heard of Ginkgo before, getting into program environment was the first challenge. It turned out that our design was very good and we hardly had to make any changes.

Overall, our project now consists of lines of Python code and lines of C++ code.

2 Changes on the Design

- We didn't implemented a matrix class, because we realized it is not useful to handle every matrix by its own. Instead we decided to handle it in numpy arrays.
- We decided to leave out the density because it wasn't
- We changed the command interface to an abstract class to reduce redundancy of the code.
- We decided to let out the possibility to select a density, because we couldn't guarantee that the fetched and cut matrices from Suite Sparse have the wanted density.

3 The Requirements

3.1 Following Requirements are accomplished

- A software that supports the described work-flow design including the embedding of external components.
- The software must be usable via a command-line interface (CLI).
- A data exchange format design that allows to store matrices and annotate them with additional meta-data, including labels.

- An extensible design for multiple entities that are able to generate matrices in the proposed exchange format.
- A dataset of at least 500 matrices in the envisioned data format and generated by the above two entities. There smallest share of matrices of a given entity must be no less than 30% of the total number of contained matrices.
- An extensible design that allows to solve the matrices using a configurable set of iterative solver algorithms using a newly developed binding to the Ginkgo linear algebra library.
- A readily implemented and trained neural network of the resNet architecture. It must be able to predict for a given matrix (in arbitrary format), which of the iterative solver algorithms is the most suitable.
- An entity that allows to store and load the trained neural network.
- The software must include entities for training and re-training a neural network from scratch, respectively from a previously stored state.
- The software must be able to show the predicted algorithm and its associated suitability probability on the standard output.
- Realization of a sustainable and quality-assured software development process. This includes a software design document, in-code documentation, unit testing and a continuous integration (CI).

Following optional requirements are accomplished:

- The software must be able to utilize GPU accelerators for the training and prediction capabilities of the neural network.

3.2 Following Requirements were accomplished as far as possible

- All mandatory requirements were as far as possible accomplished despite the cross-platformed compatibility is not fully given. This was not possible, because some used entities (ssget, ginkgo) where not Windows compatible. Compared to the specification sheet there is just the possibility to fetch and cut Suite Sparse matrices yet. As we figured out our design we realized that generating random matrices is not that easy with our knowing. So as already realized in the design document, because in Suite Sparse it is very rare to have same sized matrices from Suite

Sparse, it was not necessary to just fetch Suite Sparse matrices in one size. Instead we just implemented a generator that fetches and cuts Suite Sparse matrices.

- We decided to let out the possibility to select a density as explained in the changes of design

3.3 Following Requirements were not accomplished

- A web interface to the software that is able to select a single, a set or all matrices of an uploadable file for prediction by the neural network. The web interface may also be able to visualize the contained matrices, annotated labels as well as prediction results.
- The system must support at least five iterative solver algorithms.
- Scalability of the workflow including matrix generation, training, prediction in that multiple processors may be used in parallel.

4 Unittests

4.1 Controller

4.1.1 test_command_parser

This test checks the functionality of the command parser. It has following tests:

- dict_equal
- test_valid_input_returns_command
- test_valid_input_with_arguments
- test_valid_input_with_flag
- test_invalid_mode_throws_exception
- test_valid_collector_input

- `test_valid_label_mode`
- `test_fails_when_entering_invalid_module`
- `test_quit_with_arguments_throws_error`
- `test_collector_with_missing_optional_args_adds_default`
- `test_classify_command_with_missing_optional_arg_adds_default`

4.1.2 test_controller

This test checks the functionality of the controller. It has following tests:

- `test_controller_with_two_iterations`
- `test_invalid_input_calls_print_error`
- `test_help_flag_print`

4.2 model

4.2.1 test_collector

This test checks the functionality of the collector. It has following tests:

- `test_collect`

4.3 shared

4.3.1 test_configurations

This test checks the functionality of the loading of the configurations. It has following tests:

- `test_loading_config_values_works`

- `test_loading_config_has_right_value`

4.4 view

4.4.1 test cli output service

This test checks the functionality of the view. It has following tests:

- `test_create_observable_to_print_three_values`

5 Delays and Problems

5.1 Labeling module

Our main problem was with the Ginkgo. It was bad documented what made working with it very hard and caused a delay in our implementation plan.

First we had to find out, how to use Ginkgo and because there was not good documentation we just had examples of the repository to work with.

The next difficulty was to integrate `c++`. We didn't managed to find that out by our own, but with `ctypes` and the help of markus (he wrote us a tutorial) we could integrate `C++`.

After that we needed to figure out how to transfer the data to `C++`. With pointer in python, csr matrix format and more examples from Ginkgo repository we also solved this Problem.

The following step was to find out how the server we use works so we can find out how to use Pycharm on the server. This we got to work with a remote interpreter.

The high resolution clock function in `c++` solved our next problem: the determination of the time the solvers need.

5.2 MVC

The Basic structure for MVC was very easy to implement. Through preliminary work in the implementation phase, it was very easy to build the basic structure. However, there were some problems with integration with real modules later.

5.3 Training module

The problem with the labeling module caused a delay in the implementation of the training and classify module. testing the training / classify module, was difficult, because the data from labeling modules were needed

6 Lessons learned

First of all we thought the machine learning part of this software will be the hardest part. But it turned out to be one of the easiest. Instead of that Ginkgo was the main problem. For other projects it probably will be easier to use of a better documented library. On the other hand did we need this specific GPU accelerated solvers, so there probably would have been no better or similar solution. The same time editing of latex documents was another issue. In future it would be better to use for example ShareLaTeX and start a new line for each sentence to minimize git problems.

7 Statistics

- lines of Python code
- lines of C++ code
- commits

7.1 Work Splitting

- Collector module: Yannick and Anna
- Labeling module: Fabian and Dennis

- Training module: Yannick
- Classifier: Yannick
- Command parsing module: Simon
- Output service module: Simon
- Implementation report: Anna

8 Development model

8.1 Communication in the team

For talking about the progress and following steps the whole team met one to two times a week and another time with the tutor. Dennis and Fabian worked on the Labeler module together while Yannick and Anna implemented the Collector. Simon did the command parsing module and the output service module. As soon as the labeler module worked, Yannick implemented the training module and the classifier.

8.2 Git

Codeclimate helped to write leaner code and to take care of refactoring at an early stage

9 Glossary

Glossary

algorithm In mathematics and computer science, an algorithm is an unambiguous specification of how to solve a class of problems. Algorithms can perform calculation, data processing and automated reasoning tasks.

command-line interface A command-line interface is a means of interacting with a computer program where the user (or client) issues commands to the program in the form of successive lines of text (command lines). A program which handles the interface is called a command language interpreter.

Ginkgo Ginkgo is a high-performance linear algebra library for manycore systems, with a focus on sparse solution of linear systems.

iterative solver In computational mathematics, an iterative solver does a mathematical procedure that uses an initial guess to generate a sequence of improving approximate solutions for a class of problems, in which the n-th approximation is derived from the previous ones.

neural network The neural network itself is not an algorithm, but rather a framework for many different machine learning algorithms to work together and process complex data inputs. Such systems "learn" to perform tasks by considering examples, generally without being programmed with any task-specific rules.

resNet A deep residual network (deep ResNet) is a type of specialized neural network that helps to handle more sophisticated deep learning tasks and models.