

KARLSRUHER INSTITUT FÜR TECHNOLOGIE

FUNCTIONAL SPECIFICATION DOCUMENT (FSD)

Numerical Linear Algebra meets Machine Learning

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1 Success Criteria

Goal is 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.

1.1 Mandatory Requirements

- A software that supports the described work-flow design including the embedding of external components.
- The software must be cross-platform compatible and support at least a Linux and the Windows operating system.
- 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.
- There need to be two actual realizations of these entities, which:
 - allow to generate artificial noise with uniform and gaussian noise as well as
 - can fetch test matrices from the Suite Sparse matrix collection.
- 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).

1.2 Optional Requirements

- Scalability of the work-flow including matrix generation, training, prediction in that multiple processors may be used in parallel.
- The software must be able to utilize GPU accelerators for the training and prediction capabilities of the neural network.
- The system must support at least five iterative solver algorithms.
- 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.

1.3 demarcation criteria

- no matrices other than sparse, squared matrices will be supported
- Preferably integration of existing technologies instead of own implementation (ss-get)
- Use of Keras and Ginkgo
- The programming language Python 3 should be used
- Use of Pytest for testing

2 Product use

2.1 Scope of application

The software will be used for scientific work in the field of maths and computer science.

2.2 Target groups

Mathematicians and computer scientists who are working with sparse linear systems.

2.3 Operating conditions

- Use in the field of scientific work
- Office environment

3 Product enviroment

3.1 Software

- The product will run on Windows 10 and Linux distributions
- The labeling of the matrices and training of the neural network will be done with Linux

3.2 Hardware

- The product will run on a workstation computer
- The labeling of the matrices and training of the neural network will be done on a server with multiple GPUs

3.3 Orgware

A Documentation for the user will be generated.

4 Functional requirements

4.1 Matrix Collecting

- /F10/ Generation of sparse matrices by a given sparsity level and size
- /F15/ Generation of a given amount of matrices
- /F30/ Putting noise on the matrices
- /F40/ Saving the generated matrices in a given directory
- /F50/ Choice to either only generate matrices or to generate some and fetch some from the Suite Sparse matrix collection
- /F60/ Integration of the ssget tool

4.2 Matrix Labeling

- /F70/ Determination of the best solving algorithm by time(fix algorithms)
- /F71/ optional: Determination of the best solving algorithm by time with custom algorithms
- /F75/ Labeling the matrix with the determined best algorithm
- /F90/ Creating a grayscale sparsity pattern image of the labeled matrix
- /F100/ Saving the labeled matrix with its sparsity pattern image in a given directory

4.3 DNN Training and Testing

- /F110/ Input of matrix files from a given directory
- /F120/ Randomization of the matrix files order
- /F125/ Separation of the matrix files into a training and testing dataset
- /F130/ Existence of a neural network to train
- /F140/ Training of the neural network by a given training dataset(/F125/)
- /F141/ Testing of the neural network by a given testing dataset(/F125/)
- /F150/ Printing the accuracy(/loss) during the training and testing process of the neural network
- /F151/ optional: creating of accuracy histograms
- /F160/ Saving the neural network in its current state on a given directory

4.4 Matrix Classification

- /F170/ Input of a matrix to classify
- /F175/ Creating a grayscale sparsity pattern image of the input matrix
- /F180/ Loading a trained neural network from a given directory
- /F200/ Classification of the given pattern image by the neural network
- /F201/ Printing the classification output

5 Product data

- artificial generated matrices
- collected matrices by ssget

- 500-1000 labeled matrices for training and test
- gray scale sparsity pattern image
- neural network

6 Nonfunctional requirements

- /NF10/ All matrices are squared
- /NF20/ All fixed algorithms are used within the labeling processes
- /NF30/ The grayscale sparsity pattern all have the same size before training
- /NF40/ The NN outputs a distinct prediction
- /NF50/ The NN is saved after every iteration

7 Global test cases

7.1 the following function sequences must be checked

7.1.1 Matrix Generation

- /T10/ When generating a matrix, the returned matrix must have the right size and sparsity level
- /T15/ When generating a matrix, it must be squared
- /T20/ When generating an amount of matrices, there must be an exact number of matrices by the given amount
- /T30/ When putting noise on a matrix, the returned matrix must have noise
- /T40/ After saving a matrix in the given directory, there must be the right file, with the right format

7.1.2 Matrix Labeling

- /T50/ When labeling a Matrix, the label must be the algorithm with the shortest time needed
- /T60/ When creating a grayscale sparsity pattern image it must have the same size as the matrix and must actually be grayscale
- /T70/ After saving the labeled matrix with its sparsity pattern in a given directory, there must be a file including the right matrix, the corresponding sparsity pattern image and the right label

7.1.3 DNN Training and Testing

- /T80/ When a matrix is loaded from a given directory, the right matrix must be loaded
- /T90/ When the matrix files are randomized they have to be in a different order after every randomization
- /T100/ After separating the dataset into a training and testing dataset, the training dataset must contain more matrices than the testing dataset
- /T110/ The NN has the right input dimensions for being trained by the matrices
- /T120/ The NN is only trained by the training dataset
- /T130/ The NN is only tested by the testing dataset
- /T140/ The printed loss(/accuracy) is the actual loss of the current training(/testing) iteration
- /T150/ After saving the NN in its current state, there must be the right file in the right directory

7.1.4 Matrix Classification

- /T160/ After the input of a Matrix, the right file is loaded

- /T170/ After loading a NN from a given directory, the right NN has to be in the system
- /T180/ When printing the classification output, it has to be the prediction of the NN

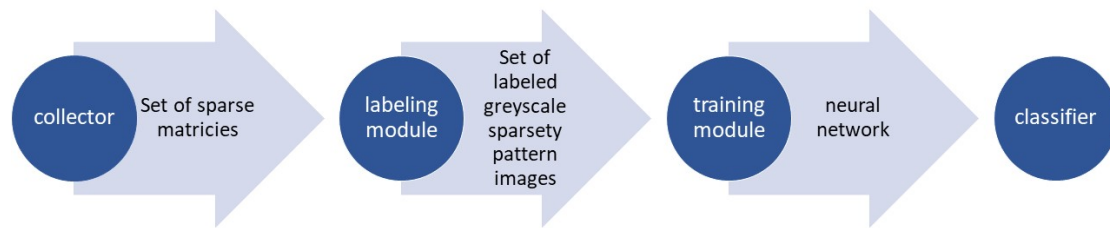
7.2 the following data consistencies must be checked

8 System models

8.1 Scenarios

8.1.1 Overview

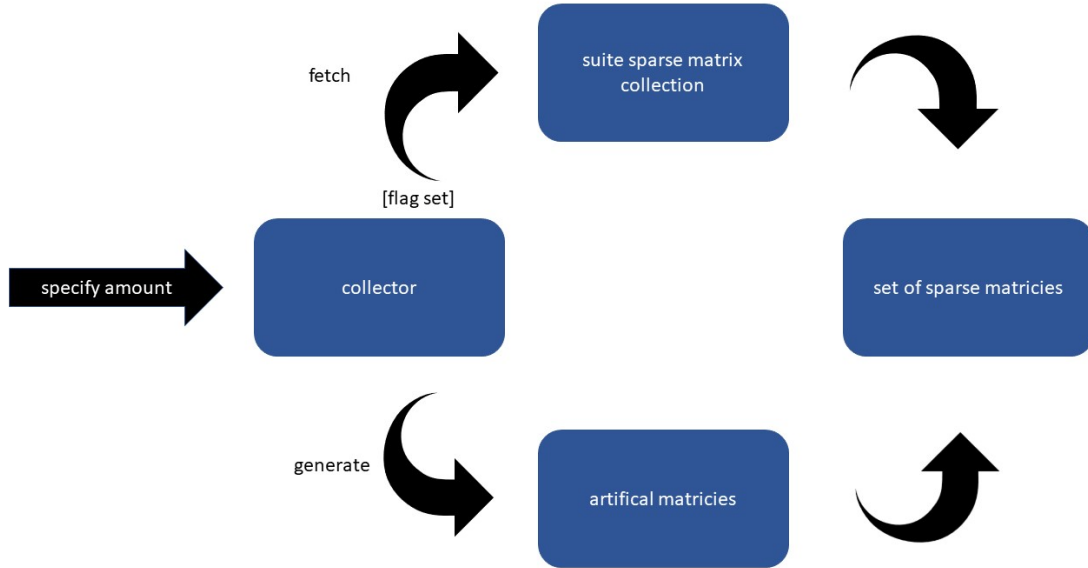
The product consists of four individual modules. The main module is the classifier . Here the user may input a sparse matrix and receive the fastest preconditioner/iterative solver combination for solving the matrix. The user may furthermore interact with the other three modules; the collector, the labeling module and the neural network. Typical interaction with those modules will be described below.



8.1.2 Use of the collector

The user wants a set of matrices for his own purpose. He likes our idea of combining the creation of matrices with fetching matrices from the Suite Sparse matrix collection. He therefore opens the module collector. He wants to generate 300 matrices of size 64x64 with a density of 0.2 and wants to use as many matrices as possible from the Suite Sparse matrix collection. He wants to call his set of matrices collectedMatrices and enters the command `collect -a 300 -n collectedMatrices -s 64 -d 0.2 -g`. When the process finished

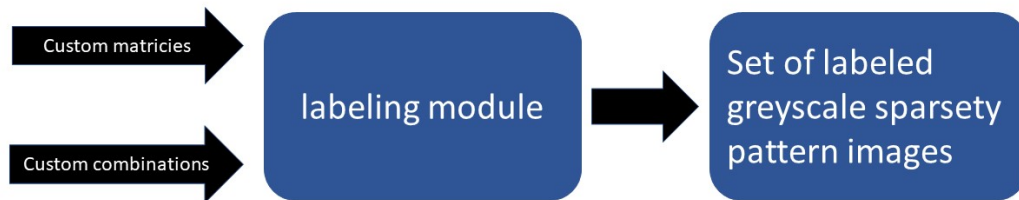
gets notified. He navigates to the results file of the collector in the file manager and proceeds to using the set of matrices for his own purposes.



8.1.3 Use of the labeling module

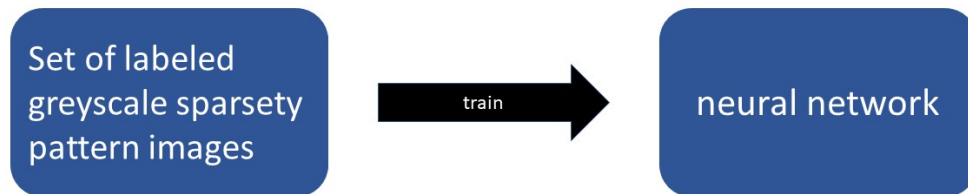
The user has a very specific problem which generates only a certain kind of sparse matrices. That is why he wants to adapt the neural network for his specific task. He furthermore only wants to use the default preconditioner/iterative solver combinations. He first of all saves all of his matrices in one directory x of his choice. Then he opens the labeling module. The command `label -p x -n labeledMatrices` will label all the matrices and generate their greyscale pattern image in the directory. The set of greyscale pattern images will be saved with the name `labeledMatrices` in the results file of the labeling module. The user may proceed with using the neural network.

Optional: The user is fine with the default matrices, but he wants to use other preconditioner/iterative solver combinations which are included in the Ginkgo library. He opens the labeling module. With the command `list` combinations he will see all the combinations that are currently used. With the command `add <preconditioner/iterative solver>` the new combinations of his choice will be added. With the command `delete <preconditioner/iterative solver>` the specified combination will be deleted. After the user made his choice he may proceed with using the neural network.



8.1.4 Use of the training module

Optional: The user has changed the set of matrices and/or the preconditioner/iterative solver combinations. He now wants to build the classifier. He opens the training module. With the command `train -n myNeuralNetwork` the neural network will be trained. The neural network will be saved in the results folder with the name `myNeuralNetwork`. The user may then proceed with using the classifier.



8.1.5 Use of the classifier

The user wants to find the fastest preconditioner/iterative solver combination for a sparse linear system. If he did not change anything in the previous modules the default settings will be used. He will first save the sparse matrix in any desired filepath `x`. Afterwards the user starts the classifier. With the command `classify -p x` - the neural network will classify the matrix and determine the fastest iterative solver/preconditioner combination for solving the matrix. This combination will be printed to the command line. (**Optional:** After determining the fastest combination the program will solve the matrix with this combination. The solved matrix will be saved in a directory the user specifies.)

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 2 & 0 \\ 9 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 12 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 1 & 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$



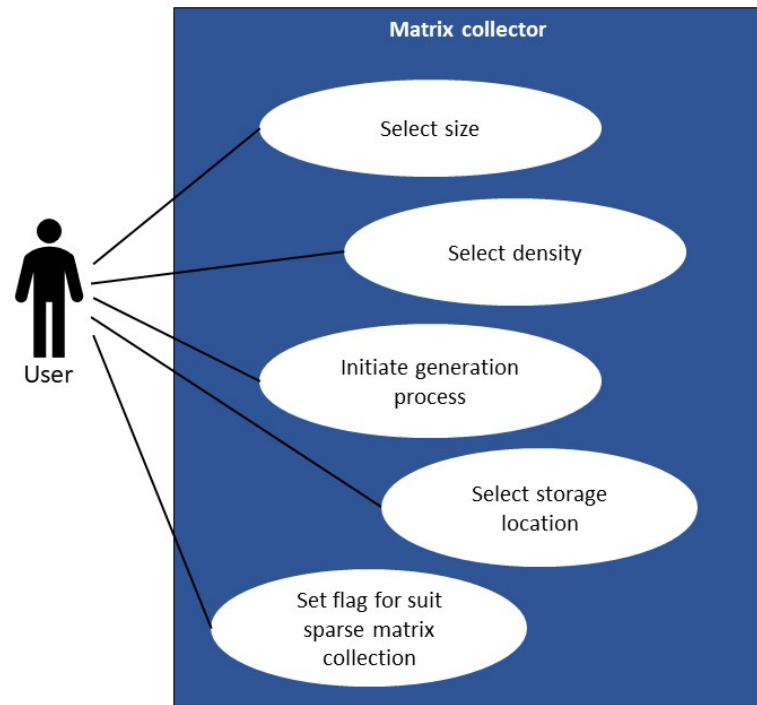
Classifier



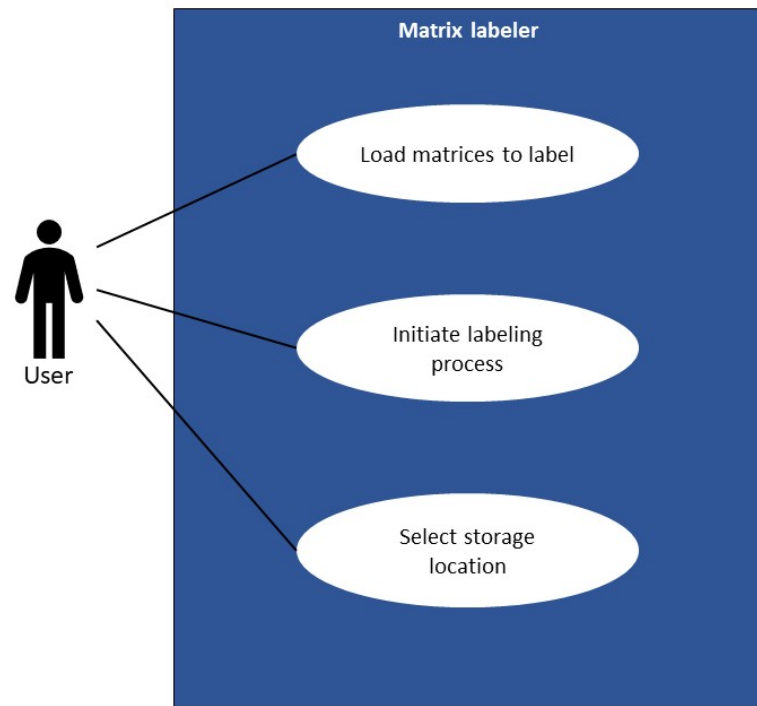
“Use preconditioner/iterative
solver combination XY”

8.2 Use cases

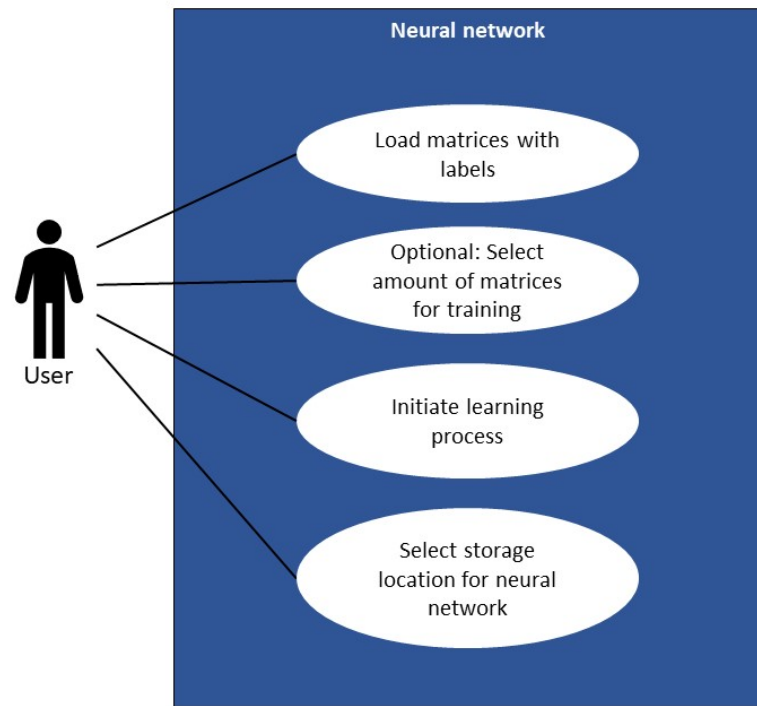
8.2.1 Matrix collector



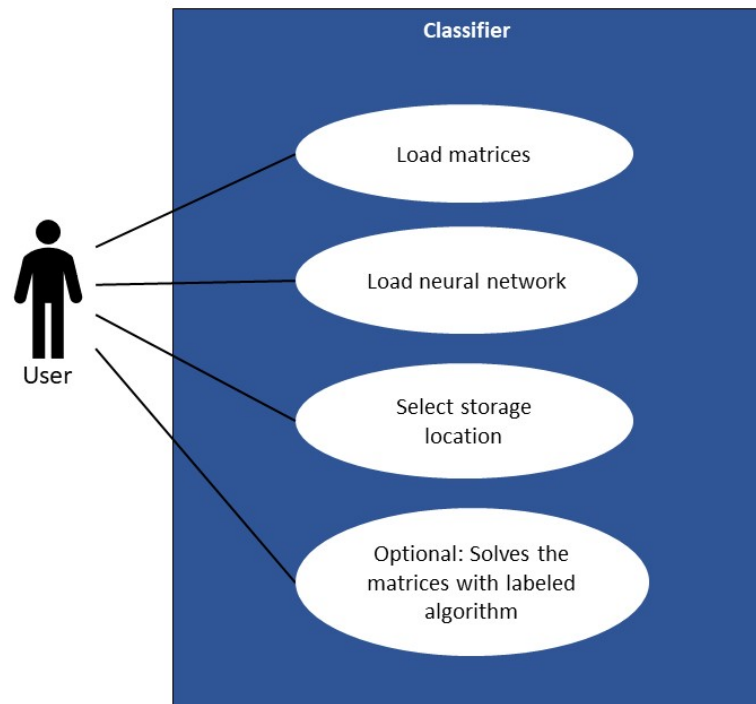
8.2.2 Matrix labeler



8.2.3 Neural network



8.2.4 Classifier



8.3 Command line options

- `/B10/collect -a <amount> -n <name> -s <size> -d <density> -p <path> -g:`
The user is able to create a specified amount of matrices that will be saved under a given name

Arguments

- `-a <amount>` Absolute amount of matrices the user wants to generate
- `-n <name>` Name under which the matrices will be saved
- `-s <size>` (optional) Absolute size the generated square matrices should have. Default is 128

- **-d <density>** (optional) Density level of the matrices. A float between 0 and 1 where 1 means no zero values
- **-g**(optional) (Flag) If set it downloads as many matrices of that size as possible from the Suite Sparse matrix collection
- **-g <path>** (optional) Path where the created/downloaded matrices will be saved

Print

- Progress notifying about the amount of matrices that are created and still need to be created
 - A message when process has finished with the path to the created matrices
 - Error, in case any required arguments are missing or invalid
 - Error, in case the specified name is already taken
 - Error, in case **-g** is set and user has no internet connection
 - Error, in case **-p <path>** is not a valid path
- **/B20/label -p <path> -n <name> -p <path>**:
The user is able to pass matrices that he wants to get labeled

Arguments

- **-p <path>** Absolute path to the matrices in the local storage the user wants to have labeled
- **-n <name>** Name under which the labeled matrices will be saved
- **-g <path>** (optional) Path where the labeled matrices will be saved

Print

- Progress notifying about the amount of matrices that are labeled and still need to be labeled
- A message when process has finished with the path to the labeled matrices
- Error, in case any required arguments are missing or invalid

- Error, in case matrices have wrong format
- Error, in case the specified name is already taken
- Error, in case the remote fetching of the matrices did result in an error
- Error, in case **-p <path>** is not a valid path
- **/B30/train -p <path> -n <name> -t <train> -p <path>:**
The user is able to pass labeled matrices to a neural network, that will learn from this matrices

Arguments

- **-p <path>** Absolute path to the labeled matrices on the local storage
- **-n <name>** Name under which the neural networks will be saved after training has finished
- **-t <train>** (optional) Float between 0 and 1. Amount of matrices used for training where 1 means all. Standard is 0.8
- **-g <path>** (optional) Path where the neural networkstate will be saved

Print

- Progress notifying about the loss of the current state based on test data
- A message when process has finished with the path to the neural network and the final loss
- Error, in case any required arguments are missing or invalid
- Error, in case matrices have wrong format or are not labeled
- Error, in case the specified name is already taken
- Error, in case **-p <path>** is not a valid path
- **/B40/classify -p <path> -n <network> -s:**
The user is able to pass a matrix to a the trained neural network, which will find the best solving algorithm.

Arguments

- **-p <path>** Path to the matrix the user wants to classify
- **-n <network>** (optional) Path to the trained neural networks, if not set, uses the neural network shipped with the program
- **-s** (optional) (Flag) If set matrix will also be solved after classification.

Print

- The preconditioner/iterative solver combination which will solve the given matrix the fastest
- (optional) The solved matrix
- Error, in case any required arguments are missing or invalid
- Error, in case the matrix has a wrong format
- Error, in case the neural network or matrix path is wrong
- (optional)/B50/**label -l**:
The user is able to retrieve a list of the available and used algorithms for the labeling module

Arguments

- **-l** (flag) If set, all other arguments will be ignored

Print

- A list of all algorithms the labeling module is able currently uses and is able to use
- (optional)/B50/**label -l**:
The user is able to retrieve a list of the available and used algorithms for the labeling module

Arguments

- **-l** (flag) If set, all other arguments will be ignored

Print

- A list of all algorithms the labeling module is able currently uses and is able to use
- (optional)/B60/**label -a <algorithm>**:
The user is able to add a algorithm that will be used for labeling matrices.

Arguments

- **-a <algorithm>** If set, all other arguments will be ignored and the algorithm will be added to the used algorithms

Print

- A message if the adding worked
- Error, in case the entered algorithm is not supported
- (optional)/B70/**label -r <algorithm>**:
The user is able to delete a algorithm from the list of used algorithms.

Arguments

- **-r <algorithm>** If set, all other arguments will be ignored and the algorithm will be removed to the used algorithms

Print

- A message if the remove worked
- Error, in case the entered algorithm is not found.

9 Glossar

Glossar

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..

classifier The last and main module in the program.It is able to determine the fastest preconditioner/iterative solver combination for a given sparse linear system. It uses the neural network trained by the module neural network..

collector The first module in the program. Responsible for generating artifical matrices and collection preexisting matrices from the suite sparse matrix collection..

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.

gaussian noise is statistical noise having a probability density function equal to that of the normal distribution, which is also known as the Gaussian distribution. In other words, the values that the noise can take on are Gaussian-distributed..

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

GPU a graphics processing unit is a specialized electronic circuit designed to rapidly manipulate and alter memory to accelerate the creation of images in a frame buffer intended for output to a display device.

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.

Keras Keras is an open source deep learning library written in Python.

labeling module The second module in the program. Responsible for executing a given set of matrices with all the preconditioner/iterative solvers combination specified. It will furthermore label each matrix with the fastest combination..

Linux Linux is an open-source software operating systems.

neural network neural networks 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..

preconditioner In mathematics, preconditioning is the application of a transformation, that conditions a given problem into a form that is more suitable for numerical solving methods..

Pytest Pytest is an alternative, more python fitting way of writing tests.

Python Python is an interpreted high-level programming language for general-purpose programming..

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..

sparsity pattern image

ssget ssget is a command line tool for downloading matrices from the Suite Sparse Matrix Collection.

Suite Sparse Suite Sparse is a suite of sparse matrix algorithms and Java interface to the Suite Sparse Matrix Collection.

training module The third module in the program. Responsible for training a deep neural network with the set of matrices and labels given by the labeling module..

Windows Microsoft Windows is a group of several graphical operating system families, all of which are developed, marketed, and sold by Microsoft..