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Accelerating BCCD using parallel computing

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Abstract

The BCCD algorithm is powerful yet computationally intensive. Even though it is highly accurate, its speed prevents the processing of larger datasets. High-performance computing solutions such as CUDA boast with massive potential speed boosts. Can high-performance computing increase the speed of BCCD to overcome the time obstruction? This thesis describes the conversion process from source code to CUDA kernel in detail. The product is a CUDA kernel that can handle exponentially larger datasets.

Contents

Chapter 1

Introduction

The BCCD algorithm, short for Bayesian Constraint-Based Causal Discovery algorithm, provides an excellent way to generate causal networks. With this algorithm the robustness of a Bayesian approach is combined with the power of a constraint-based approach. Bayesian scores are based on a large data input. These scores are then refined via reliability testing. This makes the BCCD algorithm powerful in terms of accuracy. [2] Introducing larger datasets, however, reveals a large issue. A vast amount of input results in a large or detailed amount of output. As all input needs to be processed, the time-complexity skyrockets on large datasets. This seriously limits the practical use of the algorithm, as application on large datasets would be ideal in most circumstances. This large amount of time-complexity thus limits the use of the current BCCD implementation to small datasets. [9]

To increase the size of applicable datasets the time-complexity of the algorithm needs to decrease. This can usually be done via two ways; either the code is made more efficient or the code utilises more computing power. The latter can be achieved using GPU computing. GPU computing is a rapidly growing field in computer science. [7] Not only are GPUs used to dramatically enhance computer visual performance, GPUs are also increasingly common as a way to calculate with high performance. [8] If implemented efficiently, GPUs greatly outperform similarly priced CPU systems. [10]. GPU computing thus opens up as a possible solution to the BCCD algorithm. The computational force mustered by GPUs may be able to reduce

the time constraints hampering the effective use of the algorithm [7]. This leads to the following research question: Does GPU computing increase the computational speed of the BCCD algorithm in an effective way?

The research questions can be split up using the following sub-questions:

1. How do we parallelize the BCCD algorithm using GPUs?
2. What kind of speed-up can be achieved using this parallelization?
3. Keeping the additional overhead caused by the implementation in mind, how effective is found speed-up?

Chapter 2

Preliminaries

Parallel computing is a form of High Performance computing. By using the strength of many smaller computational units, parallel computing can provide a massive speed boost for traditional algorithms.[3] There are multiple programming solutions that offer parallel computing.

Traditionally, programs are written to be executed linearly. Languages such as COBOL or FORTRAN have been designed for this linear execution. The hardware at the time did only support this linear execution. Due to this heritage, most of the programs that are written today still hold true to this linear type of execution.

With the evolution of hardware, processors have started to support multiple mathematical units. These so called "cores" allow basic parallelism to be used in traditional code. Programmes can be written in such a way that actions can be performed simultaneously; greatly improving the execution time of the program. This technique is referred to as "threading" and describes executing multiple "threads" (code executors) at the same time.

Processors have seen many improvements over time. Threading has caused a massive increase in performance for high-throughput mathematical operations. Steadily more and more transistors have found their place on processor chips. By increasing the transistor density the processors have massively increased in power.[10] All these improvements have not had any impact on usability. Processors, as central manager of the computer, have a large amount of control and autonomy over the hardware. The managing

effectiveness of the processor has only seen increase over time and has contributed even more to it's massive flexibility. Higher-level languages have become highly developed and popular, making programming easier than ever. This causes the programming of the processor, which most programming is categorized as, to be by far the most popular and practised type of programming.

More recently, parallel computing has steadily become more popular. Where for a long amount of time the power of a computer was upgraded by increasing the computing efficiency or the transistor density of the processor, newer systems sport more cores. This causes units to be more powerful, but also rely more on correctly threaded applications. New challenges in the hardware design field such as heat generation restrictions have also boosted the research into these systems. Running multiple computational units was previously frowned upon due to the increase in development complexity. Nowadays, most modern computers have at least two computational units in their processor. With the current boom in mobile hardware the development wave has been fronted by the development of low power multiple core processors. Devices such as mobile phones and tablets use these processors instead of the more traditional linear systems. The accurate division of tasks between the cores saves a monumental amount of power and greatly reduces the generation of heat. These characteristics were later found to be useful in what some may find unexpected other fields. The new Japanese exascale supercomputer manufactured by Fujitsi is rumoured to use ARM products, which is the leading developer on mobile processors.

At the heart of parallel computing is perhaps the Graphics Processing Unit. The GPU has been in development since the 1970s. Contrary to the processor, the graphics chip has been designed to work parallel from the start. This makes the GPU in design much more capable to fully utilize the advantages of parallel programmed algorithms.[7]

When using GPU's, parallel computing becomes a form of High Performance computing. GPU's have a much larger amount of cores than processors by design. By using the strength of many smaller computational units, parallel computing can provide a massive speed boost for traditional algorithms. There are multiple programming solutions that offer parallel

computing. CUDA was chosen as programming language for this research.

CUDA, Compute Unified Device Architecture, is a powerful environment that, when implemented correctly, can drastically increase the computational power available to an algorithm. To be able to implement CUDA effectively, however, the algorithm should be structured in a peculiar way. When working with devices such as graphical processing units, all information to be processed must be made accessible for these units. This means that the CUDA languages, as well as other GPU empowered programming languages, are highly subject to large memory allocation operations. As the final goal of speeding up the BCCD algorithm is to be able to process larger amounts of data, these memory allocation operations become very demanding.[9] This is why it is absolutely essential to restructure the BCCD algorithm in such a way that the memory allocations are performed optimally.

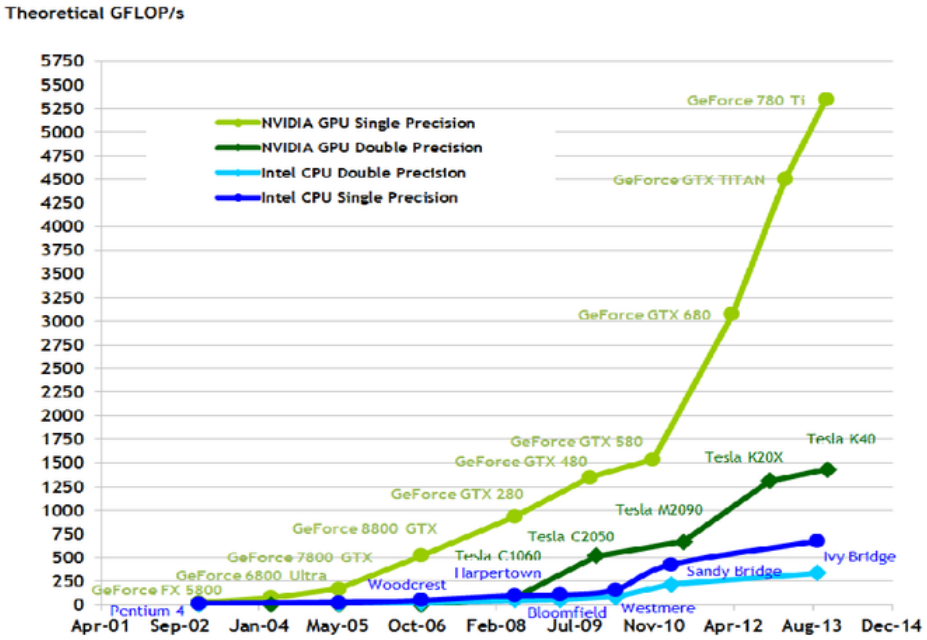


Figure 2.1: NVIDIA GPU performance compared to Intel CPU performance [3]

The BCCD algorithm is designed to run in double-precision mode [2]. This means that the calculations are done using double-precision values.

This ensures correct data handling for very accurate computations. GPU's however tend to perform much more efficiently in single-precision mode. Converting double-precision values to single-precision values is not a hazardless process. The loss in precision can cause corruption or inaccuracy in execution results. Once the BCCD algorithm has been translated to a CUDA function, a single-precision CUDA function could be attempted.

Chapter 3

Research

The translation of the BCCD algorithm to a high performance parallelized approach has been broken down to the following steps on which this research is structured:

1. Review original MATLAB version
2. Translate to Python
3. Translate to C empowered Python (SWIG)
4. Translate to CUDA
5. High performance enhancements

3.1 Review original MATLAB version

The original version of the BCCD algorithm, as fabricated by Heskes and Claassen [2], has been written in MATLAB. MATLAB is a programming language developed by MathWorks that provides an user friendly and effective workspace for scientific research. MATLAB, however, is not optimized for speed [9]. Following the research question the goal of this research is improving the speed of the algorithm using different programming techniques.

The BCCD algorithm is a multi-stage algorithm. The following stages are distinguished:

- Stage 0: Mapping

- Stage 1: Search
- Stage 2: Inference

In terms of the MATLAB code, Stage 0 is referenced to as "initialization", and stage 2 as "aftercare". In order to implement a faster version, it is essential to assess the speed of the current code per stage. The stage that performs the slowest will be the focal point. Improving on this stage will yield the greatest return. This stage will from now on be referenced to as "bottleneck stage".

As previously documented, the algorithm supposedly performs well enough on simple datasets. The datasets supplied are randomly generated multivariate gaussian model datasets with 10 variables. Increasing the amount of variables, however, quickly deteriorates the speed at which the algorithm can complete its task. This means that, to identify the correct bottleneck stage, a complex dataset has to be used. The worst scaling stage will at this point project a heavy dropoff in speed. To ascertain the projection of this trend to even more complex datasets, the duration of the tests will be compared to those of easier tests (less complex datasets).

Testing the standard MATLAB code with a dataset conjured via MVG (multivariate Gaussian model) with N=10000 reveals the following speed statistics:

D	N	Stage 0	Stage 1	Stage 2
5	1000	0.00s	0.61s	0.04s
10	1000	0.00s	13.4s	0.44s
20	1000	0.00s	40.1s	7.9s
30	1000	0.00s	108.99s	23.93s
40	1000	0.00s	169.58s	25.00s

Figure 3.1: MATLAB execution times averaged over 10 tests. Hardware specifications may be found under appendix A.

As shown above, Stage 1 consistently takes a long time to finish. To add to this, this computing stage does not seem to scale well for a higher number

D. Due to these properties, this research will focus on accelerating this part of the algorithm.

The next step is to isolate the code responsible for the execution of this stage. When looking at the original MATLAB code, a host of functions are called in order to fulfil this step. However, when looking at the execution times, a majority of the time the following function is being called:

`GetBayesianProbability_Per_Structure_BGe`

Due to the bottleneck created by this function, all attempts to improve the performance of the algorithm will be focused on this piece of code. It should be noted that, if any increase in performance is realised, this increase in performance will never be able to make the code instant. The performance increase will never be able to exceed the theoretical performance of the code when this function is instantaneous. All other functions are not altered in any way.

3.2 Target function

Python is a programming language well known for it's modularity and adaptability. Python shares many similarities with MATLAB, which allows it to be translated to relatively easily. Due to the modularity of Python and it's many possibilities, a Python version can be readily adapted for higher performance computing. This, together with the translation ease between the two languages, makes it an incredibly strong language to base future implementations on.

Pythons similarity to MATLAB is a huge convenience for the translation. Future translation to higher performing solutions will surface multiple issues. Usually, functions cannot be translated directly from MATLAB to lower level languages such as C. These languages, however, are unavoidable in order to conceive a fast algorithm. Python, however, is a very high level language and shared this characteristic with MATLAB. For most MATLAB functions a suitable Python replacement is present. In order to bridge to higher performance solutions, the next step is to make a Python version of

the algorithm. Once a Python version has been realised, Pythons modularity can be used to create better performing versions.

As only stage 1 (Search) will be translated to high-performance code, an interface has to be realised between the MATLAB version and any future versions. Any future versions will be called by a Python interface. The connection between MATLAB and future versions should thus be done by transferring the MATLAB data to a Python environment.

A ready-made solution to provide the correct environment for new versions of the algorithm is the so called exporting of the MATLAB workspace. When running any MATLAB code, any variables and values are stored and referenced in the "workspace". This workspace, combined with the execution pointer, provide all required information to run a MATLAB algorithm.

Due to these characteristics, a logical bridge between Python and MATLAB would be exporting the MATLAB workspace and loading this into Python. On MATLABs end this can be realised by using the export function

```
save(filename, variables);
```

which directly exports all listed variables of the workspace into a file. It should be noted that the save function may be called without specifying which variables have to be exported. In this case, the whole workspace is exported into the file. For this purpose, though, the variables will be specified, as not the whole workspace is required to run the algorithm. Only the variables required by the original MATLAB function call will be exported:

```
GetBayesianProbability_per_Structure_BGe(C,N,alpha_mu,T,alpha_w,SS,prS)
```

- C = covariance/correlation matrix
- N = nr. of data records in C
- alpha_mu = prior weight on precision matrix for mean
- T = parametric matrix in Wishart
- alpha_w = degrees of freedom in Wishart > (D-1)
- SS = array of structures size(C)

- prS = array of prior prob. per structure (column)

To make sure that this method of integration is suitable, it is critical to look at where this function is called in the original MATLAB code. Even more important, most certainly, is the function's effect.

GetBayesianProbability_per_Structure_BGe
Data: structure information (C,N,alpha_mu,T,alpha_w,SS,prS)
Result: scoring for given structure
initialization;
for *all structures* **do**
    set starting score;
    for *all row vectors in structure* **do**
        compute transposition key;
        calculate the determinant of the parametric matrix using key;
        calculate the determinant of the posterior parametric matrix using key;
        extend transposition key;
        calculate the determinant of the parametric matrix using key;
        calculate the determinant of the posterior parametric matrix using key;
        score the combinations;
        add score to total score for structure;
    end
    return the score for given structure;
end

Figure 3.2: The subject function

3.3 The function

The function that is isolated is a simple convergent function. It translates a large amount of input data into one output array. It takes a substructure of the chance distribution and scores it accordingly. In the code, it is called upon multiple times. This means that, if for every call the workspace is

exported to an individual file, multiple files will have to be read to interface correctly with any future implementations.

3.4 Translate into Python

In order to translate the function correctly into Python, a piece of Python script has to be written that loads the workspace values. The popular scientific calculation package Scipy provides a simple yet effective solution for this. The Scipy input-output (Scipy.io) function

```
loadmat(filename);
```

loads the workspace data into the memory. The data is stored in the standard Python List format. Individual pieces of data can be retrieved by calling their identifier.

Once the workspace is loaded into memory, all values can be easily accessed. Due to the high level structure Python has similar to MATLAB, most translation steps are fairly straightforward. This process is hereby described per part of the function:

3.4.1 Initialization

In the initialization part of the function, many of the input values are rearranged. The posterior parametric matrix R is computed and the arrays are initialized. The code in this section can be translated to Python without too much hassle. Handling the data is done by using the Python package Numpy. This package allows more advanced data manipulation. Numpy introduces Numpy arrays. This is the format the workspace data is imported in into Python using "loadmat()". Numpy will also provide future advantages in regards to interfacing with the C and CUDA versions of the code.

3.4.2 Structure loop

The structure loop consists of a double for-loop. These loop over all structures and variables inside these structures. Every structure is scored using

a formula consisting of four scoring values. Every scoring value is computed by computing the determinant of a substructure. The algorithm uses the logarithm of these determinant values in order to preserve efficiency. MATLAB has set functions for these operations, namely "log()" and "det()". These functions are standard to the MATLAB library. Python, however, does not natively support these functionalities. In order to be able to perform these operations without having to define new functions to do so, Numpy is used again. Numpy provides the functions "numpy.log()" and "numpy.linalg.det()" which behave similar to their MATLAB counterparts. Another important function is the MATLAB function "find()". This function is utilized here to form the vector for substructures that have to be analysed. These substructures are formulated using a vector which prescribes what rows and columns are to be used. A solution to translate this into Python can be found in the Numpy function "numpy.nonzero()". Both functions can be used to list the non-empty elements of a vector. This vector is then used to form the substructure in MATLAB by referencing the vector to the original structure matrix. MATLAB will return the substructure in this case. This does not translate directly to Python. Numpy, however, has the function "np.ix_()" which can be used for the same result.

3.4.3 Resolve

This fase only consists of a few lines of code. It can be as easily translated as the Initialization phase.

3.5 Improving upon the original Python version

Even though this first Python function is functional, it is far from practical. This practicality is absent in both the performance perspective and the research perspective. The new version of the algorithm performs noticeably worse than the original MATLAB version. This can likely be attributed to the code structure being written to perform well in MATLAB. The translation is rough-edged and is not optimized in Pythons favour. From a research perspective, the code can still very much be improved. The Python script is written from a very high level. Libraries such as Numpy are necessary for

a correct execution. They provide invaluable support to bridge the Python version to the original MATLAB code. The computationally intensive part, however, depends on function calls from this library to high degree. These function calls are practical to ease the translation from MATLAB code to Python code. When the Python code has to be translated into a script in a lower level language such as C, these functions lose a large amount of appeal. For example, C does not have a practical library to provide an easy yet effective parallel to the "numpy.det()" function. Once a C version has to be realised, this determinant function has to be written in C. Higher level languages such as Python are more flexible. By first writing the determinant function as a separate function in Python, the gap between the Numpy source implementation and the C function is made considerably smaller.

Before a new Python function can be realised, it is important to look at the environment the function is called in. The aim of this research is to provide a high-performing result. This means that, for this function, an implementation is preferred that performs optimally. In the algorithm, the determinant function is called to compute a determinant of a matrix of selected sizes. The size varies between a 0x0 matrix and a 5x5 matrix. To determine the determinant of a matrix the Laplace formula may be used. This formula is only practical for matrices larger than 2x2. Using the Laplace formula, the determinant is expressed in terms of it's minor, via:

$$det(A) = \sum_{j=1}^{n} (-1)^{i+j} a_{i,j} M_{i,j}$$

Where:

- A: The original matrix
- n: The size of the original matrix
- i: ith row
- j: jth column
- $M_{i,j}$: The determinant of the (n-1)(n-1)-submatrix that results from A by removing i and j

- $A_{i,j}$: The value at (i,j) in the original matrix A

The Laplace formula provides a solid way to find a determinant for any larger matrix. The formula is recursive, however, so when utilizing this formula some base cases have to be defined.

- The determinant of a 0x0 matrix is defined to be 1.
- The determinant of an 1x1 matrix is it's only value: $M_{0,0}$.
- The determinant of a 2x2 matrix is defined by the following formula:

$$\begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - bc$$

The determinant of a 3x3 matrix can be calculated using the Laplace formula. The definition of the determinant of a 2x2 matrix can be used to solve the equation. This approach, however, requires an unnecessarily large amount of operations. An extention of the 2x2 matrix definition can be used to calculate the determinant on 3x3 matrices more efficiently. The rule of Sarrus provides a more compact and usable solution to compute a 3x3 matrix:

$$\begin{vmatrix} a & b & c \\ d & e & f \\ g & h & i \end{vmatrix} = aei + bfg + cdh - gec - hfa - idb$$

A combination of the Laplace formula and the Rule of Sarrus covers any matrix larger than 2x2. The newly implemented Python function will thus utilize this to compute the determinants for these matrices. Any smaller matrix will have it's determinant derived from the listed definitions.

3.6 Translate to C empowered Python (SWIG)

Although the Python version performed marginally better than the MATLAB version, it is yet not on to par in terms of speed. To be able to achieve

higher speeds PyCuda will be implemented. This is a library for Python that allows for Python to call strong, fast CUDA kernels. These kernels are capable of achieving massive speed; even an initial version may very well outperform the original Python code. Python does not share many similarities with this kernel code, however, thus making the conversion difficult. Using a middle ground may ease the translation process. This is where SWIG, Simplified Wrapper and interface Generator, comes into play. SWIG is a powerful tool that allows the user to write a Python extension module in C. These have two important advantages over normal Python code:

1. C code is much faster than Python code, thus delivering a speed-up.
2. C code much more closely resembles CUDA code, which eases later translation steps.

There are, also, caveats to be taken into consideration:

1. C is a lower level language than Python. Many operations that have pre-built functions in Python have to be programmed from scratch in the C language.
2. The C function will be called within Python. The interfacing between the Python and the C part has to be done well in order to make the resulting code efficient.

The improved Python version greatly decreases the effort gap between a Python version and a SWIG C version. The code that has to be translated can now largely be translated directly into C code using correct SWIG interfacing.

3.6.1 The Find function

One of the most important abstractions between Python and C is the use of pointers. Python does not work with pointers. Any value accessing is done via cataloguing and variables. The Python data structure "dictionary" is a great example of this. This structure holds a list of labelled values. These labels, so called "keys", may be referenced to access underlying values. Structures like these highly contribute to the high-level nature Python has.

C does not have such a structure and instead uses a lower-level approach. This will have several implications for the C code. The two loops and their accompanied calculations require a handful of values to perform. Due to the nature of the algorithm, a large amount of the information required comes in the form of one- and two-dimensional data structures. Numpy arrays are used to both represent the structure that is being analysed and the array of scoring factors. These will all be translated to one dimensional data structures in C. An example is given below for the following Python structure:

```
matrix[i,j];
```

This details an Numpy array with size i, j. The C representation of this structure will be:

```
matrix[i*j];
```

In contrary to the Python version, the C version accesses the whole array via one index. All values are indexed as one large row of items. In this example, indexes [0 - i-1] will reference the first row of the Numpy array. The second row of the Numpy array can be accessed using the indexes [i - 2i-1], etcetera.

Perhaps the most important data accesses are those to the substructures. These substructures are defined by their row vectors. This is natively supported in MATLAB. In Python, the function "numpy.ix_" could be used as a substitute. C, however, does not provide a function for this. To be able to realise this behaviour in C, a "key vector" has to be generated. This structure is similar to the submatrix vector used in the MATLAB and Python approaches. Any data access to the substructure is done via a "key". This is an array that, for any required data access, points to the right value in the main structure. Only one such key is needed for a submatrix; in the original code the change in rows is identical to the change in columns. For example, take the following key vector:

Index	Value
0	1
1	2
2	4

When applied to the following structure:

$$\begin{vmatrix} a & b & c & d & e \\ f & g & h & i & j \\ k & l & m & n & o \\ p & q & r & s & t \\ u & v & w & x & y \end{vmatrix}$$

Will result in the following substructure:

$$\begin{vmatrix} g & h & j \\ l & m & o \\ v & w & y \end{vmatrix}$$

In the C code, this means that any time the substructure has to be accessed, the primary structure is accessed instead via:

```
matrix[key[i + n * j]]
```

Translating the MATLAB version into a Python version gave us a simple solution for the "find()" call. This function is used to calculate submatrix vector. Python provided a ready-made solution in the form of the Numpy function "numpy.nonzero()". C does not have such a set function, though, and to proceed a new C function has to be written. The function Find follows the following behaviour:

This type of behaviour is easily realised in C. The implemented solution scans the index vector. Every time a value is found that is not a zero, the output vector is appended with it's position. This results in a key that can be used for accessing the substructures.

FIND

Data: Index vector)

Result: Submatrix key array

Take the index vector.

List the positions where there is a value present (!=0).

Return this list as an key vector.

Figure 3.3: The effect of the find() function

3.6.2 Determinants

As discussed before, C does not have a determinant function in it's library. Both MATLAB and Python do have one, although the latter requires the package Numpy to do so. By creating a determinant function for the Python version, the gap between the C implementation and the Python implementation has lessened. This makes the construction of a C version almost trivial.

Only a few things have to be taken into account when translating the Python determinant function into a C counterpart:

- The matrices have been flattened in C. This means that all the indexing has to be done via one dimension, as discussed earlier.
- The substructures are to be accessed via a key vector. The original Python function has the substructure as a parameter. In the C version the parameters will contain the original structure and the key vector. All referencing has to be done via the key vector.

The determinant function written in Python was hard-coded for the first four occurrences. This means that the first four cases are calculated directly. The last two cases, 4x4 and 5x5 matrices, are computed via a recursive relationship. This keeps the code compact, but increases the amount of complexity for the system. In addition to the calculations, the computer has to perform the function calls in order to compute the right result. This is why, for the C version, a fully hard-coded approach has been chosen. This means that, in addition to the previously hard-coded cases, the 4x4 and 5x5 solution has also been hardcoded. A generator has been written to generate

the code for these operations, as the code is lengthy and repetitive, making it error-prone if coded by hand.

3.6.3 Interfacing using SWIG

After the discussed steps the C version is almost ready to go. The only thing left is actually running the function using Python. SWIG (Simplified Wrapper and Interface Generator) is used to achieve this. SWIG compiles the specified C functions into Python extensions. These extensions can be imported and called within Python.

3.7 CUDA

CUDA, Compute Unified Device Architecture, is a parallel computing platform developed by NVIDIA. The platform is designed to work with C, C++ and FORTRAN. The translation of the algorithm to a CUDA capable version can be easily achieved. The SWIG C version, being written in C, can be translated to CUDA C without too much hassle. The specific interactions required for SWIG are to be omitted and a few new interfacing actions have to be assigned to enable the execution of such a version.

CUDA is a parallel computing platform. This means that, instead of running the algorithm in a serial fashion, the algorithm should be inspected for any possible parallelisms. Doing so may greatly increase the execution speed. Multiple values could be computed simultaneously. CUDA performs this parallel execution on the Graphics Processing Unit, GPU.

The function consists of two for-loops. The outer for-loop loops over all structures, the inner for-loop over all substructures. The amount of substructures is, for a given structure, equal to it's size. This means that a 5x5 matrix will see at most five repeats in this inner loop. The outer loop, however, which specifies the amount of structures, may see a much larger amount of repeats. The amount of structures analysed this way is derived from the size of the structures. When computing on 5x5 matrices, the amount of structures analysed will be 8728, the highest amount.

Comparing the size of both loops heavily opts that a parallelization on the outer loop is the most logical, as it has the highest amounts of repeats.

Even though the algorithm is now written in a fast, parallel language, it is far from truly optimized. In the next section a few methods to improve the speed even more are discussed.

3.8 Speeding up CUDA

3.8.1 Shared memory

Algorithms programmed in a parallel way using CUDA may be fast, they are not instant. Every year the hardware on which these algorithms can be performed becomes more powerful. The raw computing force increases, allowing for more threads to be executed in parallel. Nowadays the raw computing power of the cores on this hardware is seldom the bottleneck for most algorithms. The memory management tends to play a much larger role.

CUDA knows different types of memory. The two most basic types of memory are the memory assigned to the computer itself and the standard memory assigned to the graphics hardware. Executing any algorithm on the GPU requires memory management to and from the GPU done by the computer processor itself. This tends to be relatively slow.

Memory also causes slowdown in the GPU hardware itself. When multiple threads try to access the same piece of data they are mutually excluded. The response time on these data operations depends on where the memory is that is accessed. So called "Shared Memory" is a lot faster to access than the ordinarily used Local Memory. This memory is allocated per group of threads. Any value in shared memory thus does not experience access competition from all threads. Only a small group of threads will compete for the values. In the BCCD algorithm, threads have to access the structure data many times in succession. Implementing shared memory may alleviate some of the slowdown experienced by this. It, however, does also introduce additional overhead, because the memory has to be allocated.

3.8.2 Single-precision CUDA

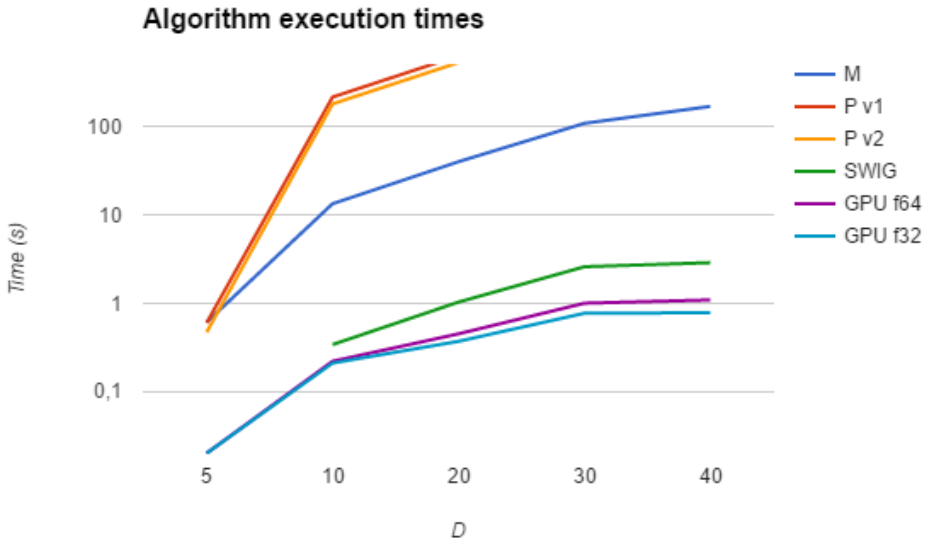
GPU computing using CUDA highly prefers single-precision. The GPU translates any computation into a single-precision mathematical operation. This means that double-precision operations are not directly supported. They are translated into multiple single-precision operations. The translation from single-precision to double-precision is simple in terms of programming. All the data types have to be simply swapped to "float". The Python interface has to convert all values to "numpy.float32". Even though creating a basic float version is simple, the conversion from double-precision to single-precision can create instability and inaccuracy in the results. The float32 version has thus only been added to demonstrate the potential speed-up to be found in this kind of conversion. In the future, a stable single-precision version could be written for the algorithm.

3.8.3 The log() function

In the current CUDA code, most complex functions have been broken down into more efficient functions. The code does however still have to compute a large amount of logarithms. Omitting these logarithms will result in wrong scoring of algorithms. It does, however, still provide a working piece of code. By comparing the speed of a version without logarithms to one with logarithms, the impact of this potentially slow function can be tested. If the difference between the two is large, the acceleration of the log() function may be a good subject of additional research.

3.9 Results

The following table contains the runtime results. For every code, the bottleneck loop has been timed. This eliminates any overhead generated by the surrounding Python or MATLAB code. The test datasets are equal to those used to initially compute the runtime of the MATLAB algorithm, as discussed earlier. Testing with datasets conjured via MVG with N=10000 reveals the following speed statistics:



D	N	M	P v1	P v2	SWIG	GPU f64	GPU f32
5	1000	0.61s	0.60s	0.47s	0.00s	0.02s	0.02s
10	1000	13.4s	216.21s	180.95s	0.34s	0.22s	0.21s
20	1000	40.1s	636.07s	531.78s	1.03s	0.45s	0.37s
30	1000	108.99s	>750.00s	>750.00s	2.59s	1.00s	0.77s
40	1000	169.58s	>750.00s	>750.00s	2.88s	1.09s	0.78s

Figure 3.4: Algorithm execution times averaged over 10 tests. Hardware specifications may be found under appendix A.

- D: Amount of variables
- N: Amount of data records
- P v1: Python using numpy.determinant()
- P v2: Python using determinant()
- SWIG: SWIG C
- GPU F64: Double-precision (original) GPU
- GPU F32: Single-precision GPU

These results show the effect a high-performance approach can have on an algorithm. When the dataset is small and uncomplicated (D=5), all versions boast respectable execution times. The high-level approaches all clock in at around half a second, while the low-level C based versions seem to be almost instantaneous. Increasing the problem size greatly increases the complexity of the problem. The high-level approaches struggle to score respectable execution times for data sets D>10. The lower-level approaches do not seem to be affected heavily. The execution times stay well under the 5 seconds regardless of which test is run.

The second Python version outperforms the first Python version. This is expected. The second version has been improved in this regard by providing a faster way to compute determinants. This function is less flexible, however, but for the algorithm this flexibility is not required.

The SWIG version competes with the CUDA versions for the fastest execution. This code does not give in at smaller dataset sizes. For larger dataset sizes the increase in execution time is absolutely affordable, yet also significantly larger than the increase the CUDA versions experience.

The difference between the two CUDA versions is extremely small. For larger datasets a few fractions of a second make up the difference, giving the lighter single-precision CUDA function the lead. The kernel launch time primarily dictates the execution time for both versions of code. This causes the difference between the two versions to be a lot smaller than initially expected.

The execution times of the SWiG version and the CUDA versions are remarkably close. To be able to assess their true relative speeds, tests on larger datasets have to be done. These tests, however, can not fit for the original testing environment. The MATLAB code and the Python versions take simply too much time to complete larger tests. This is why a new test is chosen specifically for testing these three best-performing versions.

The previous test ran on a dataset that resembled a real execution of the BCCD algorithm. For this more intensive test, however, an artificial dataset will be used. By copying the most demanding structures, the 5x5 matrices, multiple times, a so-called stress test is created. This way the code has to process a large amount of high-density structures without worrying about the smaller ones. The algorithm without the log() function and the algorithm with shared memory will also be tested. The results are shown in the following table:

S	SWIG	GPU f64	GPU f32	GPU wo log	GPU shared
500	5.19s	1.28s	0.79s	1.11s	1.21s
1000	10.70s	3.03s	2.42s	2.88s	2.78s
2500	25.91s	6.46s	3.96s	5.69s	6.18s

Figure 3.5: Algorithm execution times averaged over 10 tests. Hardware specifications may be found under appendix A.

- S: Amount of structures
- GPU F64: Double-precision (original) GPU
- GPU F32: Single-precision GPU
- GPU wo log: Logless GPU
- GPU shared: Shared memory GPU

These results provide a clearer look on the difference between the CUDA and the SWIG versions. The CUDA versions seem to perform about 3 to 5 times as fast as the SWIG version. This is a respectable increase, yet is

not a massive boost in comparison to the difference between the MATLAB version and the SWIG version. One possible explanation would be the still somewhat limited parallelization. Even though the structures are being scored in parallel, structures are subject to a maximum amount of loops. This means that the amount of realized parallelization is still limited. A possibility to enhance the speed would be to merge the scoring of multiple structures into one kernel call. This would mean that the amount of loops for a parallelization is vastly increased.

The single-precision version seems to take a larger lead in speed as the problem becomes bigger. For the GPU, any double-precision operation is split into four single-precision operations. This lead is thus expected. Both the logless version and the shared memory version perform arguably better than the original double-precision one. Even though the versions are faster, the difference is almost negligible. The log() function does not seem to have that much impact. Other memory optimizations may provide more usefull that the use of shared memory.

3.10 Overhead

The new CUDA functions provide a massive speed-up in comparison to the original MATLAB version. This test, however, did not regard any of the overhead caused by the surrounding code. This code is required to initialize the CUDA kernels and launch the algorithm. It also contains the other data operations found around the original MATLAB loops. To assess the practicality of the new version, this overhead has to be measured. The following table lists the overhead time:

D	N	GPU	GPU+
5	1000	0.02s	0.03s
10	1000	0.22s	0.29s
20	1000	0.45s	0.79s
30	1000	1.00s	1.22s
40	1000	1.09s	1.60s

Figure 3.6: GPU double-precision execution time averaged over 10 tests. Hardware specifications may be found under appendix A.

- D: Amount of variables
- N: Amount of data records
- GPU: Double-precision (original) GPU
- GPU+: Double-precision (original) GPU with overhead

Even with the additional overhead, the GPU versions provides well over a 100x speed-up in comparison to the MATLAB version.

Chapter 4

Related Work

For this research, I have visited two summer schools (PRACE Maison de la Simulation, PUMPS). Both were about the CUDA programming environment. On these summer schools, I have discussed my problem with fellow students. I also got to enjoy their projects. The interesting thing about these summer schools were that they drew applicants from all sort of fields.

The CUDA field has its fair share of host professional. CUDA, however, is primarily also a tool to be used by different researcher to increase the effectiveness of their code. This means that the people working with CUDA use it for all kinds of applications. Attending the summer schools I did not meet that many people utilizing CUDA for Machine Learning purposes. I, however, did get to know a fair share about other CUDA implementations.

CUDA is an environment that is very powerful. It can be used to great effect, but requires time to be implemented correctly. NVIDIA is slowly making CUDA more mainstream by heavily promoting the studying of it. Summer schools like I have attended provide a solid ground for students and researchers to become familiar with the technology.

Machine learning is becoming more and more popular quickly.[5] The combination of CUDA and Machine Learning is yet in its infancy.[1] The medical sector proves to be an interesting vocal point for these developments. [4] [6] Due to the popularity of Machine Learning, NVIDIA is currently heavily promoting mixing the two.

Chapter 5

Conclusions

Even though the speed-up is massive for larger datasets, the current applicability is limited. All the new versions of the algorithm use Python to load in the MATLAB workspace. This makes the current implementation too impractical. First, the MATLAB script has to be run to export all the workspace values. Afterwards, the values have to be read by the Python script. The GPU accelerated algorithm can then use these values to calculate the scores. These scores have to then be loaded into the MATLAB workspace, creating even more overhead. Streamlining this process would make the current code highly practical, yet has not been done yet due to time constraints.

Even though there are still some practical challenges to overcome, it has been proven that high-performance computing can serve as a solution for the BCCD algorithm. By locating and rewriting the mayor bottleneck in the code the BCCD algorithm has been increased in speed in a very effective way. It seems, however, that there is still performance to be gained. Most of the current performance gain is realized by more efficient, rewritten functions and the usage of a lower-level language. Parallelization has shown a fair contribution but can still be explored further, eventually creating the optimal algorithm.

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Appendix A

Appendix

A.1 A: Hardware specifications

```
OS Name Microsoft Windows 10 Pro
Version 10.0.14393 Build 14393
Intel(R) Core(TM) i7-4710HQ CPU @ 2.50GHz, 4 Cores, 8 Logical Processors
Installed Physical Memory (RAM) 16.0 GB
Total Physical Memory 15.9 GB
Available Physical Memory 6.65 GB
Total Virtual Memory 18.8 GB
Available Virtual Memory 7.32 GB

================================================================================
Device name: GeForce GTX 860M
--------------------------------------------------------------------------------
Attributes:

MAX_THREADS_PER_BLOCK:1024
MAX_BLOCK_DIM_X:1024
MAX_BLOCK_DIM_Y:1024
MAX_BLOCK_DIM_Z:64
MAX_GRID_DIM_X:2147483647
MAX_GRID_DIM_Y:65535
```

MAX_GRID_DIM_Z:65535
MAX_SHARED_MEMORY_PER_BLOCK:49152
TOTAL_CONSTANT_MEMORY:65536
WARP_SIZE:32
MAX_PITCH:2147483647
MAX_REGISTERS_PER_BLOCK:65536
CLOCK_RATE:1019500
TEXTURE_ALIGNMENT:512
GPU_OVERLAP:1
MULTIPROCESSOR_COUNT:5
KERNEL_EXEC_TIMEOUT:1
INTEGRATED:0
CAN_MAP_HOST_MEMORY:1
COMPUTE_MODE:DEFAULT
MAXIMUM_TEXTURE1D_WIDTH:65536
MAXIMUM_TEXTURE2D_WIDTH:65536
MAXIMUM_TEXTURE2D_HEIGHT:65536
MAXIMUM_TEXTURE3D_WIDTH:4096
MAXIMUM_TEXTURE3D_HEIGHT:4096
MAXIMUM_TEXTURE3D_DEPTH:4096
MAXIMUM_TEXTURE2D_ARRAY_WIDTH:16384
MAXIMUM_TEXTURE2D_ARRAY_HEIGHT:16384
MAXIMUM_TEXTURE2D_ARRAY_NUMSLICES:2048
SURFACE_ALIGNMENT:512
CONCURRENT_KERNELS:1
ECC_ENABLED:0
PCI_BUS_ID:1
PCI_DEVICE_ID:0
TCC_DRIVER:0
MEMORY_CLOCK_RATE:2505000
GLOBAL_MEMORY_BUS_WIDTH:128
L2_CACHE_SIZE:2097152
MAX_THREADS_PER_MULTIPROCESSOR:2048
ASYNC_ENGINE_COUNT:1

UNIFIED_ADDRESSING:1
MAXIMUM_TEXTURE1D_LAYERED_WIDTH:16384
MAXIMUM_TEXTURE1D_LAYERED_LAYERS:2048
MAXIMUM_TEXTURE2D_GATHER_WIDTH:16384
MAXIMUM_TEXTURE2D_GATHER_HEIGHT:16384
MAXIMUM_TEXTURE3D_WIDTH_ALTERNATE:2048
MAXIMUM_TEXTURE3D_HEIGHT_ALTERNATE:2048
MAXIMUM_TEXTURE3D_DEPTH_ALTERNATE:16384
PCI_DOMAIN_ID:0
TEXTURE_PITCH_ALIGNMENT:32
MAXIMUM_TEXTURECUBEMAP_WIDTH:16384
MAXIMUM_TEXTURECUBEMAP_LAYERED_WIDTH:16384
MAXIMUM_TEXTURECUBEMAP_LAYERED_LAYERS:2046
MAXIMUM_SURFACE1D_WIDTH:16384
MAXIMUM_SURFACE2D_WIDTH:65536
MAXIMUM_SURFACE2D_HEIGHT:65536
MAXIMUM_SURFACE3D_WIDTH:4096
MAXIMUM_SURFACE3D_HEIGHT:4096
MAXIMUM_SURFACE3D_DEPTH:4096
MAXIMUM_SURFACE1D_LAYERED_WIDTH:16384
MAXIMUM_SURFACE1D_LAYERED_LAYERS:2048
MAXIMUM_SURFACE2D_LAYERED_WIDTH:16384
MAXIMUM_SURFACE2D_LAYERED_HEIGHT:16384
MAXIMUM_SURFACE2D_LAYERED_LAYERS:2048
MAXIMUM_SURFACECUBEMAP_WIDTH:16384
MAXIMUM_SURFACECUBEMAP_LAYERED_WIDTH:16384
MAXIMUM_SURFACECUBEMAP_LAYERED_LAYERS:2046
MAXIMUM_TEXTURE1D_LINEAR_WIDTH:134217728
MAXIMUM_TEXTURE2D_LINEAR_WIDTH:65536
MAXIMUM_TEXTURE2D_LINEAR_HEIGHT:65536
MAXIMUM_TEXTURE2D_LINEAR_PITCH:1048544
MAXIMUM_TEXTURE2D_MIPMAPPED_WIDTH:16384
MAXIMUM_TEXTURE2D_MIPMAPPED_HEIGHT:16384
COMPUTE_CAPABILITY_MAJOR:5

```
COMPUTE_CAPABILITY_MINOR:0
MAXIMUM_TEXTURE1D_MIPMAPPED_WIDTH:16384
STREAM_PRIORITIES_SUPPORTED:1
GLOBAL_L1_CACHE_SUPPORTED:0
LOCAL_L1_CACHE_SUPPORTED:1
MAX_SHARED_MEMORY_PER_MULTIPROCESSOR:65536
MAX_REGISTERS_PER_MULTIPROCESSOR:65536
MANAGED_MEMORY:1
MULTI_GPU_BOARD:0
MULTI_GPU_BOARD_GROUP_ID:0
================================================================================
```

A.2 B: Double-precision CUDA kernel

```
#include <string.h>
#include <math.h>

/***
    Find function (nonzero)

    input: Array to apply nonzero to
    output; Nonzeroed array
    return: length of nonzeroed array

    e.g.
    input:  0 1 0 0 3 2
    output: 1 4 5 0 0 0
***/
__device__ int find(double *matrix, int n, int *output)
{
    int append = 0, i;
    for(i=0; i<n; i++)
    {
        if(!(matrix[i] < 0.0001))
        {
            output[i] = 0;
            output[append++] = i;
        }else output[i] = 0;
    }
    return append;
}

/***
    Determinant_transformed function
    Calculates determinant given transform key

    input: Matrix to calculate determinant of, transform key
    output: Determinant
***/
__device__ double determinant_transformed(double *matrix, int n,
    int* key, int len)
{
        if(len==0)
```

```
            return
            1;
        if(len==1)
            return
            matrix[key[0]+n*key[0]];
        if(len==2)
            return
            matrix[key[0]+n*key[0]]*matrix[key[1]+n*key[1]] -
            matrix[key[1]+n*key[0]]*matrix[key[0]+n*key[1]];
        if(len==3)
            return
matrix[key[0]+n*key[0]] * matrix[key[1]+n*key[1]] * matrix[key
    [2]+n*key[2]] +
matrix[key[1]+n*key[0]] * matrix[key[2]+n*key[1]] * matrix[key
    [0]+n*key[2]] +
matrix[key[2]+n*key[0]] * matrix[key[0]+n*key[1]] * matrix[key
    [1]+n*key[2]] -
matrix[key[2]+n*key[0]] * matrix[key[1]+n*key[1]] * matrix[key
    [0]+n*key[2]] -
matrix[key[2]+n*key[1]] * matrix[key[1]+n*key[2]] * matrix[key
    [0]+n*key[0]] -
matrix[key[2]+n*key[2]] * matrix[key[1]+n*key[0]] * matrix[key
    [0]+n*key[1]];

        if(len==4)
            return
matrix[key[0]+n*key[0]] * matrix[key[1]+n*key[1]] * matrix[key
    [2]+n*key[2]] * matrix[key[3]+n*key[3]] + ... +
matrix[key[3]+n*key[0]] * matrix[key[2]+n*key[3]] * matrix[key
    [1]+n*key[1]] * matrix[key[0]+n*key[2]];

         if(len==5)
            return
matrix[key[0]+n*key[0]] * matrix[key[1]+n*key[1]] * matrix[key
    [2]+n*key[2]] * matrix[key[3]+n*key[3]] * matrix[key[4]+n*key
    [4]] + ... +
matrix[key[4]+n*key[0]] * matrix[key[3]+n*key[1]] * matrix[key
    [2]+n*key[4]] * matrix[key[1]+n*key[2]] * matrix[key[0]+n*key
    [3]];
        return 0;
}
```

```
/***
    calculate_scores function
    Calculates the BCCD score for a probability matrix over
        subsets by key nSS.
***/

__global__ void calculate_scores(int nSS, long D, double* c0,
    double* cN, double* T, double* SS, double* R, double logpr0,
    double* logprefac, double* logps){

    int idx = threadIdx.x + blockIdx.x * blockDim.x;
    int s, pointer, i, nX;
    double logpr;                          //intermediate output
    double logTq, logRq, logTp, logRp;  //scores
    int q_i[6];
    int* translate = q_i;

    for(s = idx;  s<nSS; s+=1024) //outer
    {
        pointer = s*D;                  //"y coordinate" for
            reading dataset
        logpr = logpr0;

        for(i=0;i<D;i++) //inner, for every dimension
        {
            nX = find( &SS[(pointer+i)*D], D, translate)+1; //
                compute the map used for this iteration, this map
                 is stored under "translate"

            //nX is length of Pa_i
            //T and R are data value matrices, T is control
            //using Q_i and Pa_i, T and R are translated so that
                 a new determinant may be calculated
            //matlab and python do this by constructing a matrix
                 which is then used to point to certain values of
                 T and R e.g. t[ix(matrix,matrix)]
            //this matrix is mirrored -> only two arrays of 5
                required to sort T and R

            translate[nX-1] = i;
```

```
            if (nX > 1){
                logTp = c0[nX-1] * log(determinant_transformed(T
                    , D, translate, nX-1)); //test on P
                logRp = cN[nX-1] * log(determinant_transformed(R
                    , D, translate, nX-1)); //calc on P
            }else{
                logTp = c0[nX-1] * 0; //test on P
                logRp = cN[nX-1] * 0; //calc on P
            }
            logTq = c0[nX] * log(determinant_transformed(T, D,
                translate, nX)); //test on Q
            logRq = cN[nX] * log(determinant_transformed(R, D,
                translate, nX)); //calc on QcN[nX] *

            logpr = logpr + logprefac[nX] + logTq - logTp +
                logRp - logRq;       //compute final score
        }
        logps[s] = logpr;   //write into output
    }

}
```