**Comparative study of methods of Principal Component Analysis of automatic segmentation of functional magnetic resonance imaging (fMRI).**

Przemysław Teodorski

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Universitat Politècnica de València

1. **Introduction**

**Motivation**

In the beginning of the last decade an increase of CPU (Central Processing Unit) clock speed was generally stopped. The main reason for that is because of the thermal losses. In order to maintain continuous increase of the performance, nowadays processors comprise many cores (multicores processor). This implies that a paradigm of sequentially written programs has become unable to fully utilize this architecture. To achieve that it is necesarry to develop parallel applications i.e. applications which exploit all available cores efficiently.

In practice there are two main approaches to develop parallel applications. The first one is about processors containing several cores (2,4,6,8,…), each one (processor) processing several „heavy” threads. Another type of processors are those which contain many cores (hundreds, thousands) being able to process many „light” threads. This is how GPU (Graphic Processor Unit) works. Nowadays numerical applications with big computational complexity are implemented mainly on GPUs which are specialized for compute-intensive, highly parallel computation - exactly what graphics rendering is about - and therefore designed such that more transistors are devoted to data processing rather than data caching and flow control [1]. A low price and availability are another advantages of GPUs.

**Objectives**

The aim of this work was to implement a parallel version of PCA-based methods of segmentation of functional magnetic resonance imaging (fMRI) on CUDA (Compute Unified Device Architecture) platform in order to obtain better performance (speed-up) regarding to Matlab method’s version. The study comprises a complete documentation of the code of the implemented algorithm in CUDA C, explaining some tricks characteristc of CUDA, and other possible solutions. Later a comparison of the execution time of the methods in Matlab and CUDA are shown.

**Explanation of CUDA platform and differences between CPU**

There are some important differences between GPU and CPU architecture to consider when optimizing code. CPU cores are designed to execute instructions sequentially, so they are optimized for flow control. They have bigger cache than GPUs to minimize the memory access latency (memory bandwitdh in CPUs is generally low).

On the other hand GPUs architecture was optimized for computer games, so they contain many simple floating-point ALU executing in groups millions of instructions. The flow control is simplified. Many „light” threads are executed simultaneously, so that the memory access latency can be hidden with calculations instead of big data caches.

These features make GPUs well-suited to address problems that can be expressed as data-parallel computations – the same program is executed on many data elements in parallel – with high arithmetic intensity – the ratio of arithmetic operations to memory operations [1]. The main advantages of CUDA technology over CPU processors are memory bandwidth (byte/s) and computional throughput (FLoating point Operations Per Second).

CUDA platform consists of a host (CPU) and one or more devices (NVIDIA GPU) under host’s control. The NVIDIA GPU architecture is built around a scalable array of multithreaded Streaming Processors (SMs). A parallel application is divided into blocks of threads which are executed independently from each other. Every block is executed by one Streaming Processor, so that threads can communicate each other around the block they belong to. Communication is possible by shared memory and barrier synchronization. The partition into blocks of threads makes it possible for a scheduler to transparently scale application’s parallelism when it is run on a GPUs with a bigger number of multiprocessors (for example in the future).

NVIDIA developers named CUDA parallelism model „SIMT” (Single Instruction, Multiple Threads) which is similar to SIMD model (Single Instruction, Multiple Data). In fact threads grouped in a warp (a group of 32 threads around one block) work as SIMD models describes, but at the same time other threads from another block can execute another instruction from the same kernel program.

One of the drawback of CUDA is memory transfer between a host and a device. It is higly recommended then to minimize this, and in order to obtain speed-up a program must have enough work to do to cover memory transfer time cost.

CUDA programming platform is very powerful tool. Dependent on in what extent an algorithm can be parallelized one can easily obtain speed-up from 2 times to 1000 times and more (not limited). However it is important to identify critical points of the algorithm when parallelize it.

1. **Methods of fMRI segmentation**

**Brief state of the art in methods of fMRI segmentation**

Image segmentation plays a vital role in a medical imaging applications. Many image segmentation methods have been proposed for the process of successive image analysis tasks in the last decades.

In general, MRI segmentation is not a trivial task, because acquired MR images are imperfect and are often corrupted by noise and other image artifacts. The diversity of image processing applications has led to development of various techniques for image segmentation. This is because there is no single method that can be suitable for all images, nor are all methods equally good for a particular type of image.

The segmentation methods, with application to brain MRI, may be grouped as follows:

1. manual segmentation
2. intensity-based methods (incuding thresholding, region growing, classification, clustering)
3. atlas-based methods
4. surface-based methods
5. hybrid segmentation methods

Intensity-based segmentation methods classify individual pixels/voxels based on their intensity. In the case of the brain MRI, three main tissue classes, WM, GM, and CSF, can be distinguished based on intensity.

Thresholding is the simplest image segmentation method. A thresholding procedure uses the intensity histogram and attempts to determine intensity values, called thresholds τ, which separates the desired classes. The segmentation is then achieved by grouping all pixels between thresholds into one class. In brain MRI segmentation, thresholding can be used to separate background voxels from the brain tissue or to initialize the tissue classes in iterative segmentation methods such as fuzzy -means clustering.

Classification methods use data with known labels to partition image feature space. Image features are typically intensity values but can be also related to texture or other image properties. Classification methods can be both supervised and unsupervised. Supervised classification requires training images, which are manually segmented and then used as references for automatic segmentation of new images. One of the simplest classifiers is the nearest-neighbor classifier, where each pixel/voxel is classified in the same class as the training datum with the closest intensity.

Clustering methods are unsupervised segmentation methods that partition an image into clusters of pixels/voxels with similar intensities without using training images. In fact, clustering methods use the available image data to train themselves. The segmentation and training are done in parallel by iterating between two steps: data clustering and estimating the properties of each tissue class.

Due to the rapid development of medical image modalities, new application-specific segmentation problems are emerging and new methods are continuously explored and introduced. As a consequence, the segmentation process often becomes more complex and time-consuming. The likely future research will still focus not only on developing more accurate and noise-robust methods, but also on improving the computational speed of segmentation methods.

**Foundations and analytical derivation of the PCA method**

This section describes the foundations and applications of Principal Component Analysis (PCA) method. It is a statistical technique of identifying patterns in data, and expressing the data in such a way as to highlight their similarities and differences. Since patterns in data can be hard to find in data of high dimension, where the graphical representation is not available, PCA is a powerful tool for analysing data.

Principal component analysis procedure uses an [orthogonal transformation](https://en.wikipedia.org/wiki/Orthogonal_transformation) to convert a set of observations of possibly correlated variables into a set of values of [linearly uncorrelated](https://en.wikipedia.org/wiki/Correlation_and_dependence) variables called principal components. The number of principal components is less than or equal to the number of original variables. This transformation is defined in such a way that the first principal component has the largest possible [variance](https://en.wikipedia.org/wiki/Variance) (that is, accounts for as much of the variability in the data as possible), and each succeeding component in turn has the highest variance possible under the constraint that it is [orthogonal](https://en.wikipedia.org/wiki/Orthogonal) to the preceding components. The resulting vectors are an uncorrelated orthogonal basis set. The principal components are orthogonal because they are the [eigenvectors](https://en.wikipedia.org/wiki/Eigenvector) of the[covariance matrix](https://en.wikipedia.org/wiki/Covariance_matrix), which is [symmetric](https://en.wikipedia.org/wiki/Symmetric_matrix#Real_symmetric_matrices).

PCA can be done by eigenvalue decomposition of a data covariance (or correlation) matrix or singular value decomposition of a data matrix, usually after centring (and normalizing or using Z-scores) the data matrix of each attribute.

For PCA to work correctly it is often necessary to subtract the mean from each of the data dimensions. The mean subtracted is the average across each dimension.

**Applications.**

Principal Component Analysis is a useful technique that has found application in fields such as face recognition, image compression, and is a common technique for findings patterns in data of high dimension.

In neuroscience, PCA is also used to discern the identity of a neuron from the shape of its action potential. [Spike sorting](https://en.wikipedia.org/wiki/Spike_sorting) is an important procedure because [extracellular](https://en.wikipedia.org/wiki/Electrophysiology#Extracellular_recording)recording techniques often pick up signals from more than one neuron. In spike sorting, one first uses PCA to reduce the dimensionality of the space of action potential waveforms, and then performs [clustering analysis](https://en.wikipedia.org/wiki/Cluster_analysis) to associate specific action potentials with individual neurons.

PCA as a dimension reduction technique is particularly suited to detect coordinated activities of large neuronal ensembles. It has been used in determining collective variables, i.e. [order parameters](https://en.wikipedia.org/w/index.php?title=Order_parameters&action=edit&redlink=1), during [phase transitions](https://en.wikipedia.org/wiki/Phase_transitions) in the brain.

Finally in this work we study an application of PCA to segment fMRI images, which can be used to obtain Default Mode Network (DMN).

**A Sparse PCA**

A particular disadvantage of PCA is that the principal components are usually linear combinations of all input variables. Sparse PCA overcomes this disadvantage by finding linear combinations that contain just a few input variables.

**Introduction to the implementation of PCA method**

A Matlab pca function (standard library) is a reference implementation of this work. The implementation in CUDA bases on a code of this method. In a default mode singular value decomposition algorithm is used. An ‘economic’ version is implemented as it is more efficient and the obtained result is enough to continue executing the algorithm. It means that when singular value decomposition (A = U\*S\*VT) is calculated no columns of matrix U are computed and only the first min(m,n) rows of VT are computed.

It is worth mentioning that non-economic version might not run successfully on many GPUs as it requires a lot of memory for big datasets.

**An algorithm diagram**

A diagram of the implemented algorithm in CUDA platform is illustrated below:

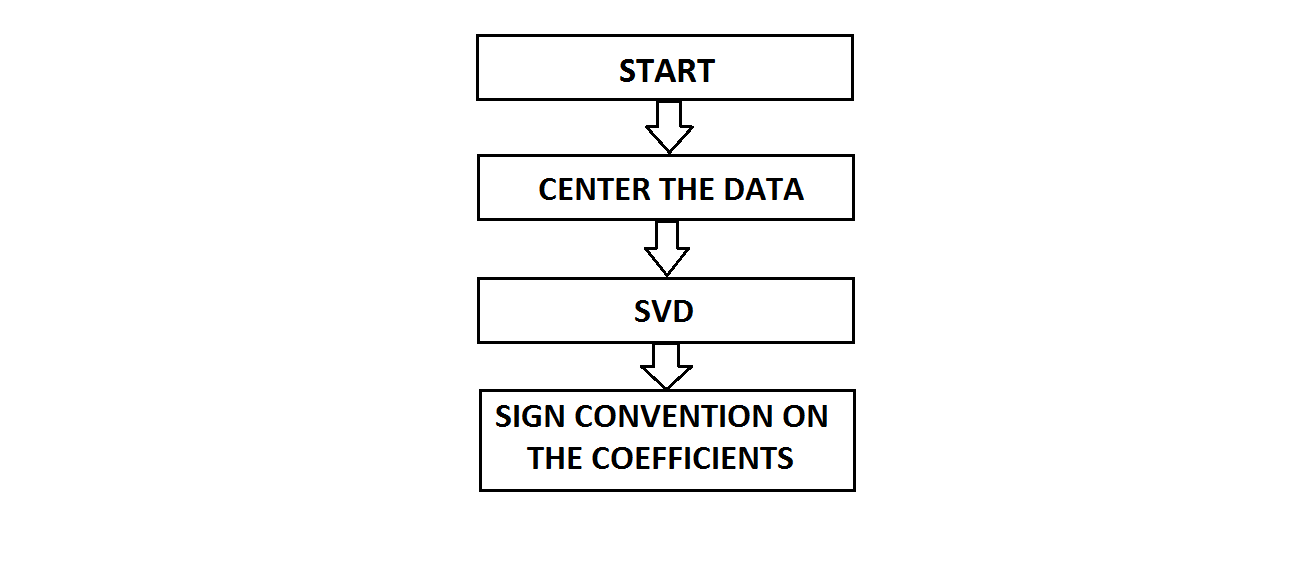


Figure 1. The diagram of the algorithm

The first step (but might be optional) in the PCA method is centring the data. Then the main part is coming which is singular value decomposition. This point is the most expensive from the computational cost standpoint. The algorithm ends with enforcing a sign convention on the coefficients (the largest element in each column will have a positive sign).

**AN IMPLEMENTATION DESCRIPTION**

A detailed description of the implemented code goes step by step from the first point of the algorithm up to the end. Later a part about memory transfer is included

The aim of this work was to achieve efficient implementation of pca method for specific problem – processing fMRI data. Therefore the code was optimized for dimensions of matrices where number of rows is much bigger than number of columns (m >> n). It might not be efficient on a data with another ratio of dimensions.

Initially the data form a matrix, where each column contains all voxels from one slice. So the number of rows m equals x\*y\*z where x,y,z are voxel’s dimensions, and the number of columns equals the number of voxels (or simply time series). The data are stored in “column-major” order.

**Centering the data**

Centring the data in this case is done by calculating an average of each row, and subtracting this average from each element of the row. The simplest scheme to calculate the average is to do sum reduction. Each row is processed by one block, so that shared memory can be used for this method.

When reading or writing to global memory in CUDA, it is highly recommended that access to the memory is coalesced. As one block processes one row, threads from the block read successive elements from appropriate row. Because the data are stored in column-major, program transposes the matrix so that global memory access is coalesced, which is very important for efficiency in case of sum reduction. Before calculating singular value decomposition, program transposes the matrix again to restore its initial form.

For sum reduction, a function using shuffle instruction was implemented. Although this version did not result in better performance (regarding to basic function with shared memory) still it needs some work to be optimized. Shuffle instruction is a powerful tool for sharing data between threads (available in GPU with Kernel architecture) and has some advantages over shared memory. It introduces a way to directly share data between threads that are part of the same [warp](http://docs.nvidia.com/cuda/cuda-c-programming-guide/index.html#simt-architecture). On Kepler, threads of a warp can read each others’ registers by using a new instruction called SHFL, or “shuffle”. It can be very useful in the future work or optimization for already written methods.

When running kernel program two configuration options need to be define by a programmer. Number of threads per block (three dimensions – x,y,z) and number of blocks in a grid (also three dimensions). Dependent on a problem size and “data shape” we can tune this options to get better performance. For example the number of threads per block should be a multiple of 32 even if the number of elements in a columns is different (smaller). It complicates a bit code (if threads instructions include reading or writing to the global memory basing on a thread index, it is necessary to check whether it exceeds an array length) but makes CUDA program being executed faster.

In case of fMRI data there is a large discrepancy between dimensions of the formed matrix. For instance in a data used in this study, the size of the matrix was 163840 x 121. Processing such data in CUDA in an efficient way is not trivial task.

As one block processes one row, we can configure kernel to have as many blocks in grid as rows. This style of kernel is known as a *monolithic kernel*, because it assumes a single large grid of threads to process the entire array in one pass (which for the GPUs used in this study this is still possible – the maximum number of blocks per grid (x dimension) is 2147483648). But instead of completely eliminating the loop when parallelizing the computation, it is more flexible approach to use a grid-stride loop. Kernel is configured to have 63536 blocks in grid, so it processes rows in a loop (number of rows in the case of using dataset is 163840).

There are some benefits to using a grid-stride loop. The first one is scalability and thread reuse. By using a loop a program is able to support any problem size even if it exceeds the largest grid size CUDA device supports. Moreover we can limit the number of block to tune performance.

Below a scheme with a matrix of data and CUDA block threads operating on a single row is illustrated:

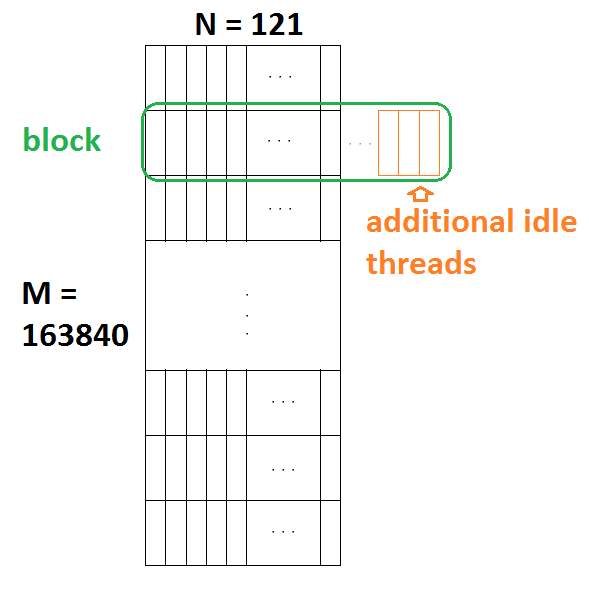


Figure 2. The sheme of CUDA processing arrays in centring the data

The number of threads in the block is a multiple of 32. If it is not equal to the number of columns, then program must check index of the each thread (because they read and write to the global memory) and dependent on it continue processing or do nothing. Simultaneously 65535 blocks are working (which for many CUDA architectures is a limit). So loop is used to cover all the rows.

**Singular Value Decomposition**

The most important (from the computational complexity and cost standpoints) part of the algorithm is singular value decomposition. A quick research of already implemented SVD method has shown that there are not many libraries for CUDA offering it. In fact CUDA API includes cuSOLVER library with SVD methods but they do not support “economic” version of the algorithm, so they are impractical for the large datasets. In this work an implementation of SVD from CULA library was used. This is the library of linear algebra methods basing on LAPACK library implementation. It supports the ‘economic’ version and works faster when m > n (the number of rows of the matrix is bigger than the number of columns). CULA routines expect that any data provided will be stored in “column-major” order. Fortunately the nifti data are stored in that way, so there is no need to transform the data.

However CULA library has not been developed since 2013, so it does not take advantage of the features new CUDA release offers. This might be a reason for writing our own implementation of singular value decomposition, but regarding available time, for this study was used the one from CULA library.

**Sign convention on the coefficients**

This task is quite similar to centring the data but in reverse. We need to span blocks of threads to process columns, not rows.

To find the largest element (absolute value) in each column of very large length (for example 163840) we cannot use ‘one block per column’ approach because the maximum number of threads per block is 1024.

The solution then is to have multiple blocks per column each one processing another part of the column. Although threads among one block can communicate each other easily, communication between blocks is very limited. In fact there are two options. One is to write results to the global memory and run as many as necessary kernel functions one after another. The second possibility is to use atomic operations. However this can be very complicated.

In the program the first option was implemented. There are multiple blocks per column each one processing its own part of the column, and writing a result to an intermediate array. This is functionality done by first kernel function. Second kernel function takes the intermediate array as an argument, collects obtained results, finds the largest element in each column, and if its sign is negative it multiplies every element in the column by -1.

This time we configure kernel’s grid to be two dimensional (see figure below describing the method). In the process of centring the data, the length of a block is large enough to cover the whole row. So we have only “a column” of blocks. In this case we have “a matrix” of blocks (which in turn covers all rows). Likewise in centring the data, a loop is necessary to process the whole length of columns.

Again when searching for a maximum element (first kernel) the global access memory is coalesced.

In order to do it in two kernel functions, the length of the intermediate array must be equal or smaller than 1024\*number of the columns. 1024 is the maximum number of threads per block and finally intermediate results from one column must be processed by one block (threads among a block can communicate each other).

Another recommendation when implementing in CUDA, is using multiplication in place of conditional branches (if else instructions). If threads of a warp diverge via a data-dependent conditional branch, the warp serially executes each branch path taken, disabling threads that are not on that path, and when all paths complete, the threads converge back to the same execution path [1].

For example when defining the sign of the largest element, instead of the following conditional if instruction:

int sign = 1;

if (max\_element < 0)

sign = -1;

we can write:

int result = max\_element >= 0;

int sign = (result == 0)\*(-1) + (result > 0);

Below a scheme with a matrix of data and CUDA block threads operating on a part of a column (first kernel program) is illustrated:

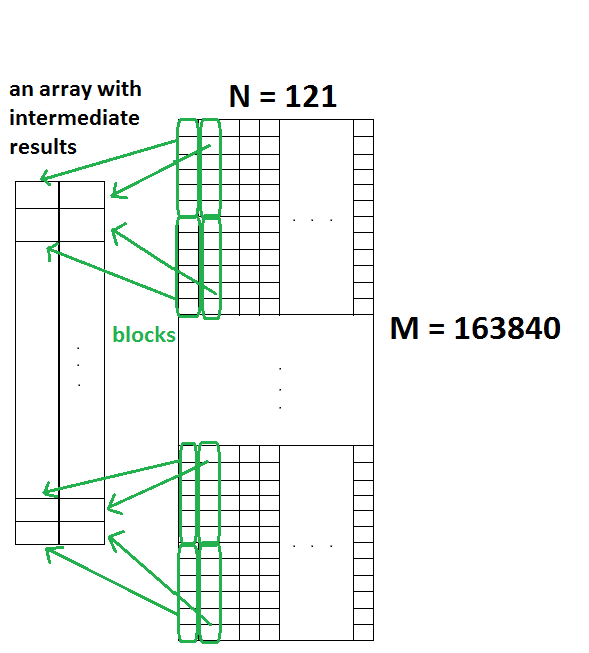


Figure 3. The scheme of CUDA processing an array in sign convention

Blocks of threads go throughout the column in a loop writing to the array (or matrix) with intermediate results. In the second dimension there are more blocks than N (again it is a multiple of 32) so only one loop is needed.

**Memory transfer**

Memory transfer on CUDA platform is a time-consuming bottleneck. To mitigate this problem one can generate data directly on GPU memory but it is not always possible. Another possibility is a pinned memory. By using pinned memory instead of pageable memory to transfer the data from a host to a device we can obtain some speed-up. On a sample of fMRI data of size 24 838 kB, transfering them by pinned memory takes on average 122 ms, whereas the same operation performed by pageable memory lasts on average 170 ms. However in some cases memory transfer over pinned memory may fail especially where the data size is too big (it depends on an operating system).

**Performance comparison between CUDA and Matlab**

GPU technical specification:

CUDA program version was tested on a GPU GeForce GTX TITAN X with compute capability 5.2. It has 24 multiprocessors each one containing 128 cores which in total is 3072 CUDA cores. GPU max clock rate is 1076 MHz.

Matlab’s script were executed on Intel Core i3-2120 CPU 3.3 GHz processor with 8 GB RAM.

Data samples were obtain from www.openfmri.org/dataset/ds000105/.

Both programs were executed ten times for a sample of fMRI data and an average execution time was calculated. The table below shows results of execution time and speed-up. CUDA execution time is a total execution time of function called on a host runPCA() – it is a CPU function, which performs memory transfer from the host to the device and calls appropriate CUDA kernel functions.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Data sample | Sample 1 | Sample 2 | Sample 3 | Sample 4 | Sample 5 |
| CUDA execution time [ms] | 2004 | 2241 | 2173 | 2112 | 2095 |
| Matlab execution time [ms] | 7680 | 8550 | 8102 | 7953 | 7891 |
| Speed-upb | 3.83 | 3.81 | 3.72 | 3.76 | 3.76 |

Generally CUDA version program was executed 3.7-3.8 times much faster than Matlab script. In CUDA program data was transferring by pageable memory, so it could be even faster including pinned memory. Nevertheless speed-up on CUDA platform is usually much bigger, but more work need to be done to optimized the code (or implement new methods).

The table below shows how much/ a part each procedure constitute of the total execution time.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Procedure | Centring the data | SVD | Sign convention | Memory transfer | Other |
| Part of the total execution time [%] | 0.18 | 84.6 | 0.02 | 8.5 | 6.7 |

It is clear that when optimizing the focus should be on SVD method.

1. **Comparative study**

**Computational cost analysis varying: mode order**

The computational cost of Principal Component Analysis method does not change with the model order. In the final part of the algorithm, it cuts all columns beginning from the value of model order and does some computations that do not influence computational cost.

**TODO – varing size of the data**

**Application: brain functional region segmentation**

**Default mode network**

The default mode network is a network of interacting brain regions known to have activity highly correlated with each other and distinct from other networks in the brain [wikipedia]. The default mode network displays more activity during rest than during task which means when a person is not focused on the outside world and the brain is at [wakeful](https://en.wikipedia.org/wiki/Wakefulness) rest, such as during daydreaming and [mind-wandering](https://en.wikipedia.org/wiki/Mind-wandering), but it is also active when the individual is thinking about others, thinking about themselves, remembering the past, and planning for the future. The netowrk activates „by default” when a person is not involved in a task.

Dysfunctional default mode network has been observed in various mental disorders, including epilepsy. For example simultaneous recording of electroencephalogram and functional MRI (EEG–fMRI) is a powerful tool for localizing epileptic networks via the detection of hemodynamic changes correlated with interictal epileptic discharges (IEDs). fMRI can be used to study the long-lasting effect of epileptic activity by assessing stationary functional connectivity during the resting-state period (especially, the connectivity of the default mode network). Temporal lobe epilepsy (TLE) and idiopathic generalized epilepsy (IGE) are associated with low responsiveness and disruption of DMN activity.

**Functional analysis of the obtained maps: model order, thresholding, statistics of slice comparison**

**TODO**

Before applying PCA method, the fMRI data should be smoothed. It is done by smoothing every slice. To segment the values returned by PCA at first we normalize them to Z scores. Then simply the thresholding segmentation method is applied. The value of the threshold was emiprically set to 2.

The data used in the study were obtained from http://www.openfmri.org/dataset/ds000115/

Below there are examples segmented fMRI images (with varying model order – number of components) showing default mode network.

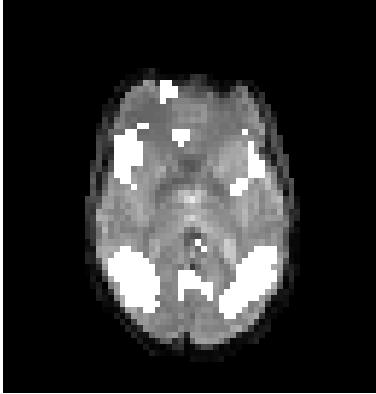
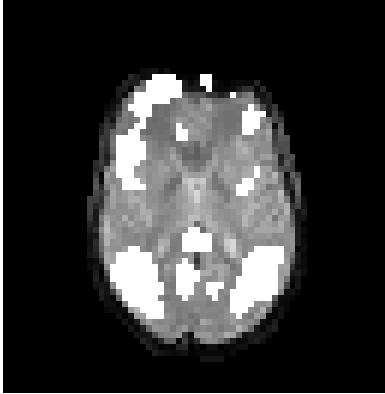
 

Figure 4a. Model order = 20,30 Figure 4b. Model order = 40

The white areas compose default mode network. For both model order values 20 and 30 the result is the same. For value of 40 method expands areas of default mode network.

**TODO**

1. **Conclusions and future work**

**Future work**

Having as a goal an improvement of the efficiency of the implemented PCA algorithm in CUDA, it might be a good idea to implement the singular value decomposition algorithm. As it was mentioned, the library used in the study is no longer developed so it does not keep up with the newest CUDA changes. Moreover our new implementation might be optimized for specific data dimension. Apart from that some new functionality may be added to implemented PCA. Especially thresholding and smoothing the data which can be highly parallelized.

In the next step an implementation of sparse PCA algorithm is considered. It has been shown that sparse PCA can extract meaningful brain parcellations. For a higher model order it can present better results than Independent Component Analysis (ICA) [3].

**Conclusions**

From the computational efficiency standpoint, a satisfactory speed-up was achieved. The parallel implementation run almost four times faster than matlab version. However still the implementation can be improved to get more speed-up. The key part to be optimized is singular value decomposition.

1. **References**

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