Random Walk with Restart (RWR) on Biological Graphs for GPUs

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July 13, 2020

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1 Introduction to the problem

Many problems in biomedicine can be defined as a ranking problem, given a set of candidate components, they are ranked relatively based on a set of known components. One example is the identification of cellular components (genes, proteins, microRNA or other molecules) that are associated with a given disease. Since the relations between known and candidate components can be naturaly represented as a graph, many network-based algorithm has been proposed. Among those, random walk with restart (RWR) has shown to be the state-of-the-art for those problems.
From an abstract perpsective RWR can be seen as multiple random walkers, each one positioned in one known component, travelling randomly through the graph but with the addition that at each itration t they have a probability of returning directly to the initial node.

Random walk with restart can be computed iteratively according to the following function

$$P_t = (1 - r)W' P_{t-1} + rP_0 \tag{1}$$

P_0 is the restart vector that represents the initial value of P (e.g. intial expression levels of a genes). r is the probability of the random walker to restart at initial position. W is the adjacency matrix of the graph $G = (E, V)$ which represents the relations between cellular components, this binary matrix W is than converted into $W' = WD^{-1}$, where D is the degree vector, which represents the probability of the random walker to go from node u to all its neighbors.
The specific value of r has little effect on the results of network propagation over a sizable range, in our case it is setted to 0.6.
At each time point t, the random walk either flows from the current node u to a randomly chosen neighbour $v \in V$ or restarts at one gene in P_0.
The propagation of P_t strictly depends on P_{t-1} and is run iteratively with sufficient step until P_t converges to a steady-state P.
Here the algorithm do not check if $P_t = P_{t-1}$ but it is repeated a fixed number of times.

2 Sequential algorithm

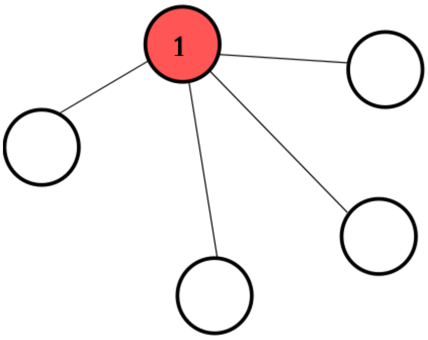
The first sequential algorithm considered performs the RWR computing iteratively formula (1) for a fixed number of steps. The sum and multiplication of the matrices are done using the library Eigen, which is a high-level C++ library for linear algebra. This runs way faster than computing all these algebric computation using nested for loop.
Since one of the major problem of performing the RWR using the matrix multiplication is the size of the matrix W another sequential was build which performs propagation using the CSR representation of the matrix W.
Since the second sequential algorithm is faster than the first, every speedup is considered with respect to the propagation using CSR.
Below it is briefly explained the concept behind the CSR propagation since it is fairly similar to the parallel algorithm.

Each iteration t can be viewed in two parts.

1. Multiplication of the $W'P_{t-1}$
2. Multiply the $1-r$ and sum with rP_0

At each time we need to store P_t, P_{t-1} and P_0 which for convenience is directly stored as rP_0. Using a CSR representation of the graph the algorithm is the following:

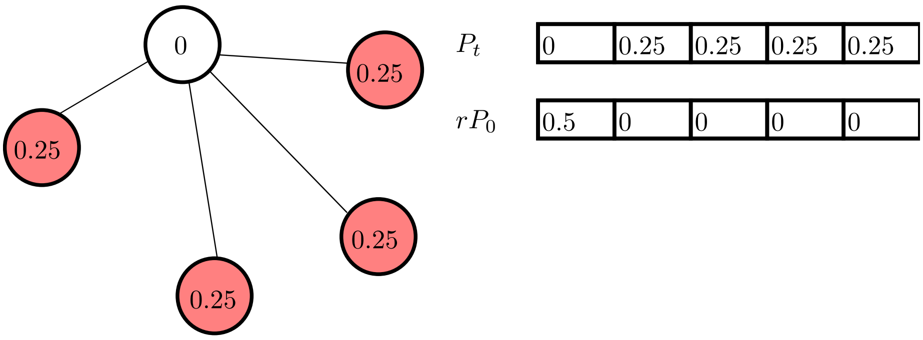
1. rP_0 is computed once at the begining of the algorithm



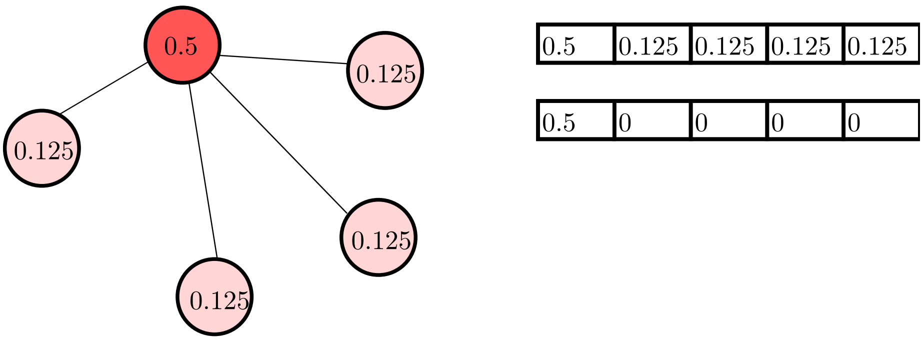
2. The value $P_{t-1}[i,j]$, which represents the propagation value in node i of patient j, is propagated in the following way

$$P_t[k,j] = P_t[k,j] + P_{t-1}[i,j]/D[i]$$

Where $k \in \text{Neighbours}(i)$ and D is the degree of node i.
Then $P_t[i,j] = P_t[i,j] - P_{t-1}[i,j]$.
Using the analogy with the random walker: the more neighbours a node has, the less is the probability of walking to that neighbour.
The second part is instead given by the fact that the random walker cannot remain in its node.



3. When all nodes have propagated they are multiplied by $1 - r$ which is the probability of not restarting to the intial condition and then summed with $rP_0[i, j]$.



3 Parallelization in cuda

The following three groups of kernels (1,3,5) represents the progression to the final speedup, which is achieved through kernel 3 + kernel 5.
Kernel 1 is the first attempt to parallelization, using a similar algorithm of the sequential. It uses a frontier that represents all the nodes different from 0 at time t but has many atomic operations which are necessary for the result.
Kernel 3 reduced the number of atomic operations and uses virtual warp, this improves the perfomance but still lack the use of shared memory for reason that I am going to explain below.
Kernel 5 use the shared memory performing the propagation of a single patient on a single block in sequential, this is faster but can be done only for small graph (in my case less than 2000).
The final parallelization is done by employing kernel 5 when the number of nodes fit into the shared memory and in all other cases Kernel 3.

3.1 Kernel 1

The first attempt to parallelization is similar to the sequential descripted above. It contains 3 kernels, each one representing one of the steps that were mentioned in the CSR sequential.

1. **InitKernel**
   This kernel creates in parallel, for a given patient, the rP_0. If the initial value is different from 0, it sets a flag for node i to 1.
   This flag is than used to create the frontier nodes that needs to be propagated.

2. **PropagationKernel**
   This is the kernel that performs the propagation of the nodes.
   Since each node needs to update its neighbours and also other nodes maybe updating the same neighbour the sum must be done using `atomicAdd`.
   In order to check if a node was already in the frontier or it is new the control over the `flag` is atomic (`atomicCAS`) and also the counter of nodes in the frontier is atomic.
   All of these needed atomic operations slow down the process.

3. **RestartKernel**
   The multiplication of $(1 - r)$ and then sum rP_0 is performed in a separate kernel since we need to be sure that all nodes have propagated.

3.2 Kernel 3

This is the final kernel which is used to execute the RWR.
It is divided into two kernels and it does not use a frontier.
The idea behind this kernel is that instead of propagating each node to its own neighbours, each node query the neighbours and update itself, in this way all this atomic add operations on its neighbours becomes only a memory access.
At each time all the nodes are updated with their neighourbs, this could waste some time in the first iterations but it was assumed the following:

1. Nodes propagated quickly even starting with the matrix full at 10% wasting only the first few iterations.
2. When we perform propagation on a gene expression matrix many genes have an expression different from zero.

The first kernel compute rP_0 as before without computing any frontier.
The second kernel instead propagates each node using only one `atomicAdd`.
This kernel also use the concept of **virtual warp** which means that each Warp is divided by `VWARP_SZ` in order to better deal with the diversity in the degrees of the graph and coalescing memory access of the `VWARP_SZ` consecutive edges.
This kernel do not exploit shared memory since I was not able to tile in anyway the graph, e.g. if my shared memory length is 1024, nothing prevents the node 11 to have as neighbour the node 1025.
For this reason kernel 5 was developed, which exploit shared memory, but it can be used only when there is a small number of nodes.

3.3 Kernel 5

Since we cannot have only part of P_t and P_{t-1} in the shared memory, this kernel store them entirely but can be used only when the size of the shared memory of the block is less than the size of nodes.
E.g. with my GeForce GTX 1050 Ti the maximum number of nodes is near 2000.
The idea of this kernel is that each block performs in sequential only one patient. Sequential in this case means that each block performs in parallel a portion of the propagated vector of a single patient, using virtual warp, and then proceed to the rest of the vector.
Here we do not get rid of the `atomicAdd` but in newer graphic card `atomicAdd` on the shared memory performs faster than in global memory.

4 Testing

Tests have been performed using random graphs and biological graphs on a GPU GeForce GTX 1050 Ti and CPU Intel(R) Core(TM) i7-8750H CPU @ 2.20GHz.

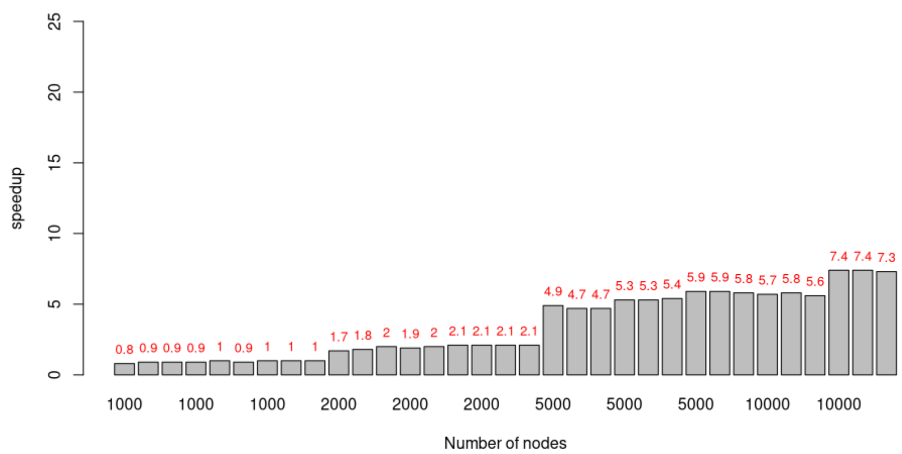
4.1 Random graph

The first tests are done using random graphs and random mutation matrix (binary matrix).
The edge list is randomly generated starting from a number of nodes and the density of the graph (or the average number of degrees) using the Erdős-Rényi algorithm.
The mutation matrix are generated given a number of patients and the density of the matrix.

4.1.1 Kernel 1 Vs Sequential

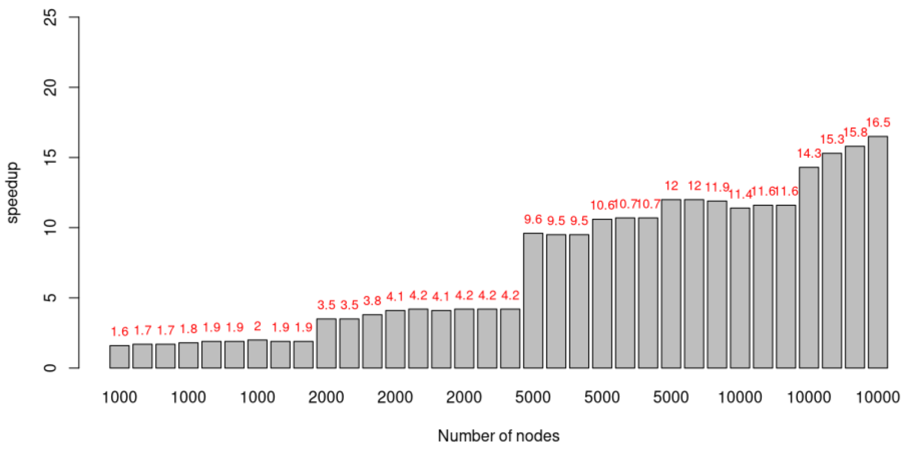
The following histogram show the speedup of the Kernel 1 with respect to the sequsequential.
Each propagation is characterized

- Number of nodes (1000, 2000, 5000, 10000)
- Density of the graph (0.2, 0.5, 0.8)
- Density of the mutation matrix (0.1, 0.5, 0.8)



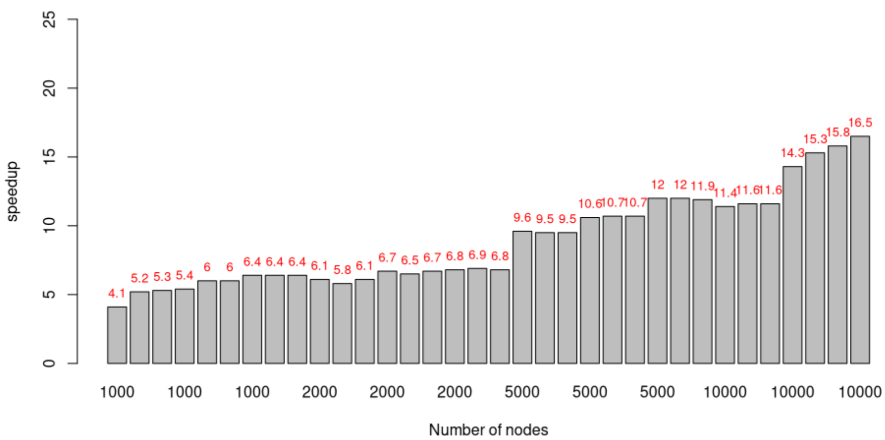
The most influential parameters is the number of nodes. Even if Kernel 1 depends on the mutation matrix density, given a graph with 20% of edges present, the frontier tend to fill up quickly.

4.1.2 Kernel 3 + 5 Vs Sequential



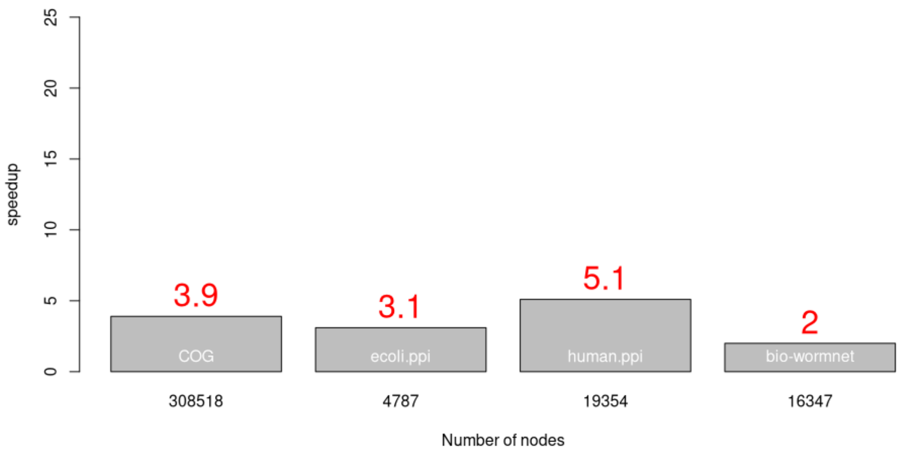
Here we can see that increasing the density of the graph we also have a speedup. This is beacuse the input depends not only on the number of nodes but also on the number of edges, e.g. when number of nodes equals 5000 and the density of the graph is 0.1 there are roughly $3 * 10^6$ edges, instead with a density of 0.8 there are $5 * 10^6$ edges.
The speedup of Kernel 3 with respect to Kernel 1 is in general 2x.

Since we can use the Kernel 5 up to a certain number of nodes here is the final speedup on random graph given by Kernel 3 + Kernel 5.

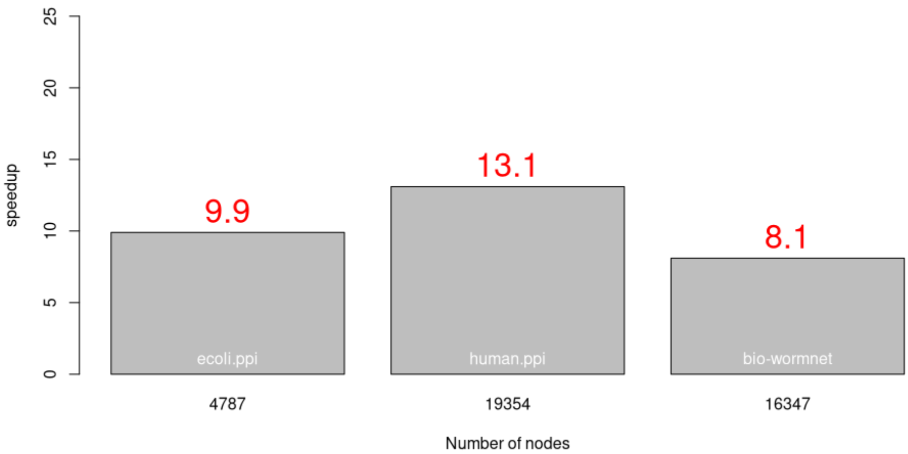


4.2 Biological graph

The speedup in the biological graph is not as high as the speedup of the random graphs.
This is mainly due to the fact that biological graphs are way more sparse and do not follow any specific distribution, while the degrees of the random graphs presented above generally follows a gaussian distribution.



In order to test the hypothesis of the gaussian distribution I have constructed for each biological graph a corresponding synthetic graph with the algorithm used for random graphs.



Also using the profiler `nvvp` I have checked the **warp execution efficiency of the kernel** in both the biological and the artificialy biological graphs and they are respectively 44% and 81%.

5 Conclusion

The presented parallelization of RWR can reach up to 16.5x of speedup for graphs that follows a gaussian distribution but is not able to reach those speedup for biological graphs, having a peak of 5x.
On the other hand this approach is able to perform RWR parallel using the CSR representation of the graph while most of the RWR implementations need to load the whole adjacency matrix.