PERFORMANCE GAIN FOR CLUSTERING WITH GROWING NEURAL GAS USING PARALLELIZATION METHODS

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Keywords: Neural net, Growing neural gas, Parallelization.

Abstract: The amount of data in databases is increasing steadily. Clustering this data is one of the common tasks in Knowledge Discovery in Databases (KDD). For KDD purposes, this means that many algorithms need so much time, that they become practically unusable. To counteract this development, we try parallelization techniques on that clustering.
Recently, new parallel architectures have become affordable to the common user. We investigated especially the GPU (Graphics Processing Unit) and multi-core CPU architectures. These incorporate a huge amount of computing units paired with low latencies and huge bandwidths between them.
In this paper we present the results of different parallelization approaches to the GNG clustering algorithm. This algorithm is beneficial as it is an unsupervised learning method and chooses the number of neurons needed to represent the clusters on its own.

1 INTRODUCTION

Knowledge Discovery in Databases (KDD) is the process of preparing and processing data, and afterwards the evaluation of the results that emerged from that data. In the processing step of KDD often includes a clustering. When using neural networks, in the training of these networks much time is spent, especially when many neurons are used and huge amounts of data have to be processed. Neural networks cannot be utilized with too much data, as the training would not finish in acceptable time. Parallelization seems to be a way to minimize the computing time, needed for such a training.

Modern computing platforms often comprise a huge number of processing units. CPUs as well as GPUs (Graphics Processing Units) (Szalay and Tukora, 2008) and small desktop clusters (Reilly et al., 2008) are examples for these platforms. They are more and more in the scope of high performance computing. With their huge amount of computing units it seems reasonable to compare different parallelization approaches with regards to how they scale with an increasing degree of parallelism.

In our work we use the GNG algorithm, first introduced by Fritzke (Fritzke, 1995). The GNG offers the possibility to only give an upper bound on the number of neurons. It decides for itself, if that number has to be exhausted. After the learning phase the connections between the neurons indicate clusters of data vectors in relative proximity to each other. This clustering property is then used in the ICIx (Görlitz, 2005), a new data base indexing structure.

2 RELATED WORK

Other approaches have been undertaken to parallelize neural networks. Especially the longer known SOMs (Kohonen, 1982) have been in the scope of these efforts. In Labonté (Labonté and Quintin, 1999) the neurons were distributed on different computers. It was found, that for large numbers of neurons a nearly linear speedup can be achieved. However, we do not use that huge numbers of neurons but their results can be an orientation for our work.

Another work has been done by Ancona (Ancona et al., 1996). He examined parallelization on Plastic Neural Gas networks. In these special networks the dependencies between the neurons are not as strong as in GNG networks. He distributes the training data vectors on different computing nodes which each hold only a fraction of the hole network. Through a special update strategy he achieves a speedup in the number of computing units used.

Another way to speed up especially hierarchical

Adam A., Leuoth S., Dienelt S. and Benn W. (2010).
PERFORMANCE GAIN FOR CLUSTERING WITH GROWING NEURAL GAS USING PARALLELIZATION METHODS.
In *Proceedings of the 12th International Conference on Enterprise Information Systems - Artificial Intelligence and Decision Support Systems*, pages 264-269
DOI: 10.5220/0002903502640269

clustering is shown by Görlitz (Görlitz, 2005). His clustering method first does a coarse grained clustering. Afterwards, the found clusters are further split up. This can be easily parallelized by distributing the first partition to as many nodes as clusters were found. It has been shown, that the discovery of the first partition is the bottle neck of this method. We are searching for ways to speed up each learning step. That does not touch the ability to distribute our approach with this method.

Cottrell (Cottrell et al., 2008) shows a way to do a batch learning with a neural gas network. There the adaption of neurons only takes place after certain steps of presentation of data to the neural net. During these batches the neurons do not interact with each other. Thus these regions of the algorithm offer a source for parallelism. We ran tests using this method. The results are also shown later in Section 4.

3 GNG-ALGORITHM

The goal of the GNG algorithm is to adapt a net of neurons $\mathcal{A}$ to represent the distribution of a given data set $\mathcal{D}$. The data records in that set are presented to the neurons. The neurons then adapt their internal reference vector to that of the given data record. After a certain amount of steps λ, new neurons can be inserted or removed from the net. Neurons can have edges between them, signaling that they belong to a cluster. A cluster represents an area of the data space with the records contained in it are relatively similar. The formula symbols used also later on are shown in Table 1. For a listing and further discussion of the algorithm see (Fritzke, 1995).

3.1 Non-parallel Runtime

An adaption of that algorithm is used for the results in this paper. This variant does not remove neurons from the net to speed up the growth. It also decreases the adaption rates when an integer multiple of λ cycles is near. The last change has no impact on the overall complexity of the algorithm and will be not further regarded. The first one decreases the computing time and simplifies the formulas later on.

The runtime of the single steps of the GNG algorithm as found in (Görlitz, 2005) is shown in Table 2.

In (Adam et al., 2009) we already showed that the runtime for one step of the learning algorithm is linear in v and d. When accumulated over all steps, it shows that the overall runtime is lineary depending on d, λ and $|\mathcal{D}|$ but is quadratic in $|\mathcal{A}|$.

Table 1: Symbol definitions.

symbol	description	estimated size
$\lvert\mathcal{D}\rvert$	number of data records	millions
$\lvert\mathcal{A}\rvert$	maximum number of neurons	typically 2-100
v	number of neurons per step	2 to $\lvert\mathcal{A}\rvert$
d	dimensionality of the records and reference vectors	up to 1500
λ	insert and remove interval for neurons	ca. 100
p	number of processing units used	1-500

Table 2: Runtime components for non-parallel case.

step	runtime
compute distances	$v \cdot d$
finding winner and second	v
insert edge	1
actualize error	d
actualize winner	d
actualize neighbors of winner	$v \cdot d$
adjust multiplier	2

3.2 Data Parallelization

Figure 1 shows the scheme we used for our data parallelization approach. The data is partitioned and the partitions then are learned by different independent GNGs. After a certain amount of steps, these nets are merged. Several synchronization or merge strategies may be applied, particularly the following three were used in this work:

1. *Average:* This method takes two neural nets and does a position based average of the neurons weight vector.
2. *Batch:* Another variant is to not move the neurons during the training phase and accumulate their movement in a variable Δ_i for each net i. Out of these Δ_i an average is computed and this average is applied to the neurons of the distributed nets.
3. *GNG:* The GNG algorithm itself can be applied for the merge of two nets. The neurons of one net are the data vectors the training of the other one. Due to a cubic term we do not regard this method further for our runtime estimations.

The equations for the runtime can be found in (Adam et al., 2009). They show that a linear speedup in the number of used computing units can be expected.

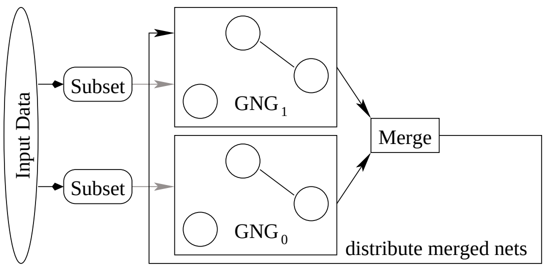


Figure 1: Data parallelization scheme.

3.3 Neuron Parallelization

The neuron parallelization scheme is depicted in Figure 2. The neurons of the GNG are distributed to different computing sites. The winner and second is chosen in parallel and then all nets adjust their corresponding neurons to the new input. In (Adam et al., 2009) we showed, that the expected speedup is linear in the number of computing units that are used.

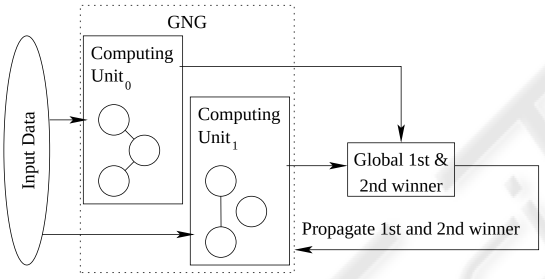


Figure 2: Neuron parallelization scheme.

4 EXPERIMENTAL RESULTS

We will now present the results of our work. First we give an overview of the speedups gained with the different parallelization methods on CPU and GPU. After that we take a short look on the quality of the data parallelization with regards to the utilized merge strategy. For all tests the network parameters shown in Table 3 were used.

As CPU we used an Intel®Core2 Q6600 (Quad Core) processor at 2.4 GHz with 4 GB of DDR2-800 RAM. The GPU was an Nvidia GeForce 8800 GTX SLI system with each graphics board equipped with 768 MB of GDDR3 RAM and a shader clock of 1350 MHz. The operating system was Windows Vista in the 64 bit variant.

Table 3: Network parameters for the GNG learning.

insert interval	λ_{ins}	= 10
winner adaption rate	ε_b	= 0.1
neighbor adaption rate	ε_n	= 0.002
error normalization value	α	= 0.001
dimensionality of the data records	d	= 96
maximal neuron number	$\lvert\mathcal{A}\rvert_{max}$	= 32

4.1 CPU-results

We started our tests using a CPU implementation. Table 4 shows the results for the—theoretically better—data parallelization. The last line shows the theoretical speedup. Above it is the real speedup gained. Synchronization between the nets was done right before inserting of a new neuron. It can be seen clearly, that the speedup using the simple average method is the best. It is nearly linear. A graphical representation can also be found in Figure 3.

Table 4: Data parallelization computing times in seconds.

	merge method	# threads 1	2	3	4
runtime	average	5.8	3.1	2.1	1.6
	batch	5.8	3.3	2.3	1.9
	GNG	5.8	3.4	2.5	2.2
speedup	average	1.0	1.9	2.8	3.6
	batch	1.0	1.8	2.5	3.1
	GNG	1.0	1.7	2.3	2.6
speedup	theoretically	1.0	2.0	3.0	4.0

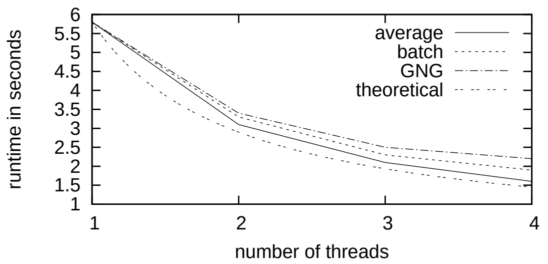


Figure 3: CPU Runtimes.

Table 5 shows the results using the neuron parallelization approach. Barriers were used to synchronize the different threads. The speedup—even without measuring of the barriers—is not as big as at the data parallelization. Including the barrier time, this is because of the synchronization between the network fractions that has to be done at every single data presentation. The speedup without the barriers is not as good as the theory would predict. One reason for this is, that the synchronization is not done parallelly. Also, the serial components of the algorithm might be larger than expected.

Table 5: Neuron parallelization computing times in seconds.

#neuron threads	1	2	3	4
without barriers	5.8	3.7	2.6	2.3
with barriers	5.8	10.0	14.7	17.3
barrier overhead	0.0	6.3	12.1	15.0
speedup				
without barriers	1.0	1.6	2.2	2.5
with barriers	1.0	0.6	0.4	0.3
theoretical speedup	1.0	2.0	3.0	4.0

So we conclude that on sole multi-core CPU systems the data parallelization approach is not only theoretically but also practically the most promising one.

4.2 GPU-results

The second test environment were GPUs. For the Nvidia GPUs we had at our disposal, the CUDA framework is the programming toolkit to use. Some limitations exist for the parallelization on these GPUs. The structure of the GPU is so that only distinct partitions of the processing units can communicate efficiently with each other. These partitions are called streaming multi processors (SM) by Nvidia. The SMs themselves consist of thread processors, that run the actual computations. Neuron parallelization can only happen inside such an SM due to this limitation. (NVIDIA Corporation, 2009)

Further the GPU has dedicated memory areas, especially shared, constant, and global memory. The constant respective texture memory are cached portions of the global memory. The shared memory is inside the SMs. These SMs also have a common register set for all thread processors inside. The single memory types are summed up in Table 6. Due to the limited amount of memory, the maximum number of neurons was 32 and the length of the vectors was limited to 96 inside one SM.

We used a hybrid parallelization due to the limitations on the GPU. We distributed the data on different SMs. Each SM then trained its own independent net. The nets were synchronized using synchronization methods described in Section 3.2. Inside each SM we parallelized the neural net with neuron and vector parallelization. Due to its complexity the CPU computed the synchronization with the GNG-merge.

Table 6: Different memory types on Nvidia 8800 GTX GPU.

type	size	speed
constant	$\leq$ 64kB	fast (cached)
global	whole memory	slow (uncached)
shared	16kB (16 $\times$ 1kB)	fast, inside SM, comparable to registers
registers	8192 per SM	very fast

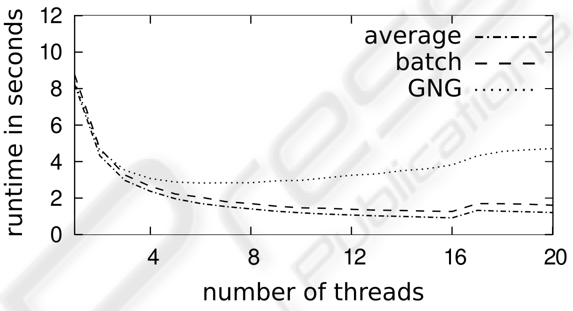


Figure 4: Runtimes for parallelization on GPU.

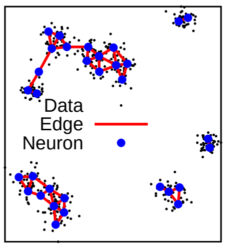
Figure 4 shows the final runtimes of the parallelization using a mix of data, neuron, and vector parallelization. It can be seen clearly, that using only the neuron and vector parallelization, the GPU is slower than the CPU implementation (one data thread). When the data parallelization is added, the runtimes on the GPU fall below that of the CPU. Newer GPU generations have even more computing units, so further speedup is expected.

4.3 Clustering Quality

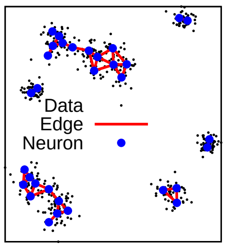
The quality of the clustering was also of special interest to us. That is because the data parallel approach alters the result of the algorithm. As starting point we took the original non-parallel variant of the GNG algorithm. We presented the same input data, originating from Fritzke (Fritzke, 1995), to all algorithms. Figure 5a shows the results of the non-parallel variant. The clusters are well covered by the neurons.

The results of the batch variant are shown in Figure 5b and present the best merge method—in therms of clustering quality—up to this point of our research. The clusters are not as well covered as in the non-parallel variant of the algorithm, but still show the structure of the clusters.

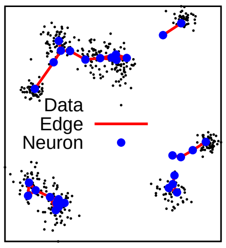
We also evaluated the merge methods—using again the GNG algorithm and the average value of the



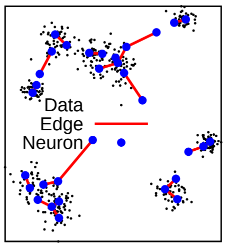
(a) original GNG



(b) batch-merge GNG



(c) GNG-merge GNG



(d) average-merge GNG

Figure 5: Training results.

neurons. Their results are shown in Figures 5c and 5d. The GNG-merge lets the neurons collapse. This is because for the merge only the reference vectors of the neurons are used. At the beginning of the training, these vectors are in the center of the data vectors and are not adapted fast enough to later represent the data vectors. The average-merge scattered the neurons and broke up clusters. This is because the neurons are merged according to their number, not their position. So neurons belonging to different clusters could be merged. For the GNG-merge, we will try to alter some of the parameters to get better results, but for now the batch-merge is our favorite.

To measure the quality of the clustering, different methods were proposed. We used the Dunn (Dunn, 1974), Goodman-Kruskal (Goodman and Kruskal, 1954), C (Hubert and Schultz, 1976), and Davies--Bouldin (Davies and Bouldin, 1979) index. The quality of the clustering only changes when data parallelization is used. This is the only method that changes the original GNG algorithm. In our cases this meant a decrease—depending on the merge method—of the clustering quality.

Using the Goodman-Kruskal index all merge methods are near the optimum of 1, only the GNG method (using 16 data threads) is slightly worse. This means that pairs of neurons inside one cluster mostly have smaller distances between them than pairs of neurons of different clusters. The other index operating on the distances between neurons—the C index—showed no differentiation. The GNG method again showed a slightly worse behavior at 16 data threads.

The Dunn index, stating that clusters are well differentiated, is overall low. The best values for this index are gotten with the non-parallel algorithm. Then using data parallelization the batch merge method showed the best results at approximately 0.15 (values greater than 1 are good).

Finally the Davies-Bouldin index was used. It is a measure for the compactness of the clusters in relation to their distance. The batch and the GNG merge method are at the level of the non-parallel GNG algorithm. Only the average merge method showed deteriorating values with an increasing number of data threads.

5 CONCLUSIONS

We have shown, that—theoretically and also practically—a performance gain of the GNG algorithm through parallelization can be achieved. Data parallelization has the most potential but also has its pitfalls in the synchronization methods used. We also showed that for the used GPU architecture a further sub-parallelization on neuron and vector level is advantageous.

We will further explore the possibilities of the parallelization of the GNG algorithm with regards to other parallel architectures such as clusters. The upcoming multi-core CPUs and GPUs, which promise much larger numbers of computing units are in our focus, too. (Intel, 2007) (Kowaliski, 2007) (Etengoff, 2009) (Sweeney, 2009)

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