Effects of Pooling in ParallelGlobal with Low Thread Interactions

Dániel Zombori and Balázs Bánhelyi Department of Computational Optimization, University of Szeged

Keywords: black box, stochastic, global optimization, parallel computing

Received: March 31, 2020

The first step toward a new version of Global is discussed. It is a fully distributed algorithm. While the proposed implementation runs on a single machine, gossip based information sharing can be built into and be utilized by the algorithm. ParallelGlobal shows a feasible way to implement Global on a distributed system. Further improvements must be made to solve big real world problems with the algorithm.

Povzetek: Predstavljena je nova verzija algoritma Global z imenom ParallelGlobal.

1 Introduction

Global is an optimization algorithm built from multiple modules working in an ensemble. While older implementations viewed the algorithm as a whole, the most recent GlobalJ framework handles algorithms as a collection of interlocking modules. GlobalJ has several implementations for local search algorithms and variants of Global. Main characteristics of the single threaded version were established in [4]. In recent years Global was further developed [6] and it has several applications [5, 7] where it aids mostly other research works. To speed up optimization processes we developed an algorithm [1] that is capable of utilizing multiple computational threads of a single machine. It cannot be directly implemented for distributed systems as the millisecond order of magnitude latency in communication would significantly slow down the synchronization of threads. To mitigate this problem we propose Parallel-Global, a parallel implementation suitable for distributed systems with high latency or even with unreliable communication channels. In this paper we introduce an experimental version whose main purpose is to test the feasibility of the proposed solution. It provides an algorithm skeleton for a real distributed implementation.

2 Global

Global is a global optimizer designed to solve black box unconstrained optimization problems with a low number of function evaluations and probabilistic guarantees [1, 2, 3, 4, 6, 8, 9, 11]. It uses local search algorithms to refine multiple sample points hence Global is a multi-start method. Global also utilizes the *Single Linkage Clustering* algorithm to make an estimation about the values of samples from the aspect of optimization.

2.1 Updated global algorithm

While the updated Global algorithm has only minor changes and in a lot of cases performs equally to the original, it is superior in execution order, therefore we consider it as the basis for improvements.

Global has an iterative framework where samples in an iteration compete with samples of previous iterations. The original version contains four phases in every iteration consisting of sampling, reduction, clustering, and local search. In the updated algorithm the clustering and local search phases are merged by an implementation which alternates them.

Algorithm 1 GLOBAL

1: while termination-criteria() is not true do $S \leftarrow S \cup \{uniform(lb, ub) : i \in [1, new \ samples]\}$ 2. $S \leftarrow sort(F(s_i) < F(s_{i+1})), s_i \in S$ 3: 4: $R \leftarrow \{s_i : i \in [1, reduced \ set \ size]\}$ $S \leftarrow S \setminus R$ 5 while R is not \emptyset do 6: for $C\ {\rm in}\ clusters\ {\rm do}$ 7: $d_c \leftarrow \left(1 - \alpha^{\frac{1}{|clustered| + |R| - 1}}\right)^{\frac{1}{dim(F)}}$ 8: 9٠ $N \leftarrow \left\{ r_i : d_c > \left\| r_i - c_j \right\|_{\infty} \land F(r_i) > F(c_j) \right\}$ if N is not \emptyset then 10: 11: $C \leftarrow C \cup N$ $R \leftarrow R \setminus N$ 12: 13: repeat iteration 14: end if 15: end for $l \leftarrow local\text{-}search(r_1 \in R)$ 16: $\begin{array}{c|c} argmin \\ C \in clusters \\ c/10 & c. \end{array} & \left\| l - argmin F(c_i) \right\|_{c_i \in C} \end{array}$ $C_l, d_{min} \leftarrow argmin$ 17: 18: if $d_{min} < d_c/10$ then 19: $C_l \leftarrow C_l \cup \{l, r_1\}$ 20: else 21: $clusters \leftarrow clusters \cup \{\{l, r_1\}\}$ 22: end if 23: $R \leftarrow R \setminus \{r_1\}$ end while 24: 25: end while

Algorithm 1 describes the updated Global in detail. In lines 2-5 the algorithm performs the sampling phase. Selection of sample points is random, using uniform distribution in the search space. The generated samples are placed in container S which has a list structure. To find the most promising samples, S is sorted and a reduced set of samples is acquired with the lowest function values. R contains the reduced set, which is removed from S.

When samples are ready to be processed, in lines 6-24 the algorithm alternates between clustering and local searches while there are unprocessed samples left. At lines 7-15 samples in R are tried against the clustered samples. To determine if $r_i \in R$ is part of cluster C we need the distance threshold d_c . This depends on the dimension of the objective function, the number of samples currently known in the clustering process, and the $\alpha \in [0, 1]$ parameter. The latter controls the decrease speed of d_c while more samples are added, in order to adapt to the expected decrease in distance between two random samples. With d_c set, sample pairs $(r_i \in R, c_i \in C)$ are evaluated to determine if r_i is part of C. The two criteria are having a clustered sample c_i with function value lower than r_i and it being closer with the infinity norm (Manhattan distance) than d_c . Samples in R satisfying both of them are moved to the current cluster C. When a point is clustered, all samples in R can potentially be clustered too, therefore $r_i \in R$ is rechecked against C. After the for cycle finished, samples in R cannot be the part of an existing cluster, therefore performing a local search is inevitable.

Local searches are performed in lines 16-23, where l is the local optimum reached from r_1 . To determine if l is a newly found local optimum, a comparison with the cluster centers is needed. The center of a cluster is the sample in the cluster with the lowest function value. By finding the cluster with the closest center the algorithm can decide whether the optimum is already found. If the distance d_{min} to the cluster C_l with the closest center is lower than a tenth of the d_c threshold, it is considered to be the same local optimum. In this case l and r_1 are added to C_l , otherwise they form a new cluster. Since r_1 is either in an already existing cluster or in a newly created one, we can remove it from R. The while loop in lines 6-24 repeats until Rbecomes empty. With no unclustered samples left Global finished an iteration. The number of executed iterations is limited by the termination criteria.

3 ParallelGlobal

Our goal is to derive an implementation from the updated Global which is multi-threaded with few interactions between threads. The necessity for few thread interactions comes from the fact that on huge scale optimization tasks a single computer is not sufficient and in multi-computer environments the communication between machines is relatively slow compared to inter-thread communication. We address this problem by removing the synchronization of computational threads and replacing it with a message based information sharing scheme. D. Zombori et al.

We can view ParallelGlobal as a naive parallelization of Global. The main idea lies in the parallel execution of Global iterations, while sharing information between computational threads. Consequently, inter-thread communication is necessary, however only a few selected data containers have to be shared. Also, the shared containers have independent data points and no deletions, therefore inconsistencies cannot arise from data insertions. These considerations make the algorithm for distributed systems viable. Luckily information gathering techniques of Global can be maintained with messaging, therefore results almost always apply to ParallelGlobal as well.

3.1 ParallelGlobal worker

Algorithm 2 describes the ParallelGlobal worker which is the implementation of a single computational thread. The worker might run on a machine by itself, or multiple workers can use the multi-threaded environment of a computer.

Algorithm 2 ParallelGlobal
1: while termination-criteria() is not true do
2: exchange-data()
3: $S \leftarrow uniform(lb, ub)$
4: $R \leftarrow reduce(S)$
5: $d_c \leftarrow \left(1 - \alpha^{\frac{1}{ clustered +1-1}}\right)^{\frac{1}{dim(F)}}$
6: for C in clusters do
7: $N \leftarrow \{r_i : d_c > r_i - c_j _{\infty} \land F(r_i) > F(c_j)\}$
8: $C \leftarrow \dot{C} \cup N$
9: $R \leftarrow R \setminus N$
10: end for
11: $r_{min} \leftarrow argmin F(r_i)$
$r_i \in R$
12: $l \leftarrow local-search(r_{min})$
13: $C_l, d_{min} \leftarrow \underset{C \in clusters}{argmin} \left\ l - \underset{c_i \in C}{argmin} F(c_i) \right\ _{\infty}$
14: if $d_{min} < d_c/10$ then
15: $C_l \leftarrow C_l \cup \{l, r_{min}\}$
16: else
17: $clusters \leftarrow clusters \cup \{\{l, r_{min}\}\}$
18: end if
19: end while

Similarly to Global, ParallelGlobal also runs in a loop to complete iterations until a termination criterion is met. Unlike Global, the new algorithm needs a data exchange step (line 2). At the start of every iteration, received messages can be processed and new messages can be sent according to a suitable policy. The messages contain evaluated data points arranged into clusters. These clusters can be handled as if they were evaluated locally by clustering the center point (minimizer point) of the cluster. If the center point corresponds to an existing cluster, the two clusters should be merged while duplicate points are filtered out. Otherwise, the received cluster describes a previously unknown local optimum and it can be added to the existing clusters without modifications.

Lines 3 and 4 perform sampling and reduction. In previous Global versions sampling and reduction was performed by taking a randomized sample set, then using a sorted sample pool and taking the best samples out. ParallelGlobal cannot utilize efficiently a fully synchronized common pool due to the distributed nature of the system. In this version we envisioned simple solutions providing a similar effect to a shared pool. Also with more complicated solutions closer approximates are possible. The evaluated implementations are discussed in Subsection 3.2.

In lines 5-10 the clustering occurs. It is very similar to the original clustering algorithm. The only change is that we know that no more than one sample is in R. This is also true for the local search (lines 12-18) which is identical with the local search part of the original.

3.2 Current implementation

The current implementation of ParallelGlobal only simulates the described functionality with some simplification. First, it runs on a single machine with multiple threads as a single program. Second, messaging is simulated by synchronization on the given containers while they are written, but reading operations happen simultaneously. During clustering, the cluster list is only read to a point determined before the process starts, hence new clusters will be excluded from already started searches. This also resembles the effects of messaging, like delays and losses in information spread. Because no real messaging is present, the exchange-data() function is only a placeholder for now.

To evaluate the differences between Global and Parallel-Global in more depth, we implemented the latter with two kinds of *reduce()* functions. The naive pool-less implementation ignores the *reduce()* function, in every iteration it creates a sample that is evaluated with clustering, and then (if not clustered) with local search. The 'pooled' implementation simulates the sample pool and reduction by generating a local pool. Along with Global, we use the notion of the sample reducing factor. Global generates a number of samples and takes a fraction of that number from the common pool. Pooled ParallelGlobal creates samples such that one sample has to be picked according to the fractional reduction.

Beyond these pooling and sample reduction strategies much more exist, for example taking a single sample every iteration and using random sample reduction, possibly aided with spatial measures on the samples information value. A more complex but possible solution would be a distributed sample pool. Samples could be transferred between local pools over reliable data connection. This would ensure that a sample is only evaluated by a single worker and would create a bigger variety of samples to choose from.

4 **Results**

The algorithms were examined from two aspects; comparison in the number of function evaluations and scaling of run time with additional threads. Numerical results were obtained on the following functions, definitions can be found



Figure 1: Numeric results of the poolless version on the Shubert (left) and Spikes (right) functions.

in [10]. Ackley, Discus, Easom, Griewank, Levy, Rastrigin, Schaffer, Schwefel, Shekel-5, Shekel-7, Shekel-10, Shubert, Spikes¹, and Zakharov. For the evaluations we used two termination criteria, the maximum number of function evaluations is 10^5 which is a soft condition therefore overshoot is possible. To check whether an optimum point is reached we use the expression

$$|F(x^*) - F(x)| < 10^{-8} + |F(x^*)| \cdot 10^{-6},$$

where x^* is a known global optimum point and x is the point in question. To emulate computationally more expensive functions we defined the hardness level. A hardness level of H means that the function will be evaluated for 10^H microseconds at the requested point. Please note that microsecond level timings can be inaccurate and only have effect in trends, while at the millisecond scale the timings show the real 10x factor.

Global is a stochastic optimizer, moreover Parallel-Global is also affected by the operating system's thread scheduling, consequently run times and the number of function evaluations can differ largely from one optimization process to the other. To reduce the noise induced by this, we obtained data points by averaging the results of 100 runs with every configuration. The algorithm parameterizations were identical except for the number of threads.

On the left side of Figure 1 we show results for Poolless ParallelGlobal on the *Shubert* test function, namely the number of function evaluations (NFEV) and the speed of the optimization process (1/runtime), both relative to Global. On the horizontal axes we see the number of

¹Spikes function definition:

$$f(x) = \begin{cases} 1000, & \text{if } \|x - (15.25, 15.75)\|_2 \le \frac{1}{4} \\ 1002 + \prod_{x_i} \sin(2\pi x_i), & \text{otherwise} \end{cases}$$

threads. The vertical axes show the number of function evaluations and optimization processes run in unit time respectively, both divided by the result of Global on a single core. H0 to H3 denotes the hardness value for the given data series. Shubert is a function with many local optima and a flat global trend. In case of Global, NFEV is mostly in the [500, 2000] range with an average of 900. On the top-left graph relative NFEV shows that we have an increase with a factor of two. On a single thread the multiplier of $2^1 = 2$ shows that the algorithm is by itself inferior to Global. This static multiplier is explained by the lack of a sample pool which could reduce the necessary number of local searches. They give the bulk of the NFEV and while Global uses 5 local searches on average ParallelGlobal needs much more, around 18. The dynamic growth is also explained by the local searches, combined with multi-threading. Finding the global optimum with local search takes several function evaluations in sequence. Since multiple threads start local searches independently, more evaluations can happen until one of them reaches the global optimum. Moreover when the optimum is found, the program does not terminate immediately, all local searches have to finish. This phenomenon increases the NFEV due to the intrinsic usage of multi-threading and local searches.

The bottom-left subgraph of Figure 1 shows the speedup with additional threads and different hardness values. While for H0 and H1 the additional threads caused a slow-down due to synchronization time and increased NFEV, on computationally more demanding versions we achieved a significant speedup. The results are promising because for the hardness value of 3 on a single thread a function evaluation took only 1ms on average. With higher evaluation times, the additional computational power would have more effect.

On the right side of Figure 1, we show the results for the *Spikes* test function which also has many local optima and a flat global trend. Poolless ParallelGlobal suffers from the lack of a sample pool on the *Spikes* function too. On the other hand, no dynamic change in NFEV is experienced. Without a sample pool ParallelGlobal had a much harder time finding the global optimum, which would often exceed the 10^5 NFEV limit. This resulted in close to constant NFEV and saturation of threads only on low hardness values. Based on the relative speed graph, we gain speed linearly with additional CPU power on higher hardness levels. Since the function is very cheap to evaluate and ParallelGlobal has to do much more evaluations, only H2 and H3 gives an advantage to the multi-threaded implementation.

On the left side of Figure 2 we show results for Pooled ParallelGlobal on the *Shubert* and *Spikes* test functions. As before the NFEV and execution speed is examined, relative to the same data on Global.

Pooled ParallelGlobal halved the NFEV on one thread, then grew to 16 times the single thread value. This phenomenon is independent of hardness, and hence curves closely match on the top-left subgraph. The single thread NFEV is halved because Global takes a set of 400 sam-



Figure 2: Numeric results of the pooled version on the Shubert (left) and Spikes (right) functions.

ples in every iteration and then uses another 400 samples to find the optimum summing to 800 NFEV. Pooled Parallel-Global takes only 27 samples per iteration and also needs around 400 samples to find the optimum summing close to 400. The NFEV almost exactly grows with the number of threads, pointing to the failure of job parallelization in a way when effectively the same job is done by every thread. This is supported by the fact, that for this configuration the number of local searches matches the number of threads, and hence no parallelization is possible. This happens on functions where the optimum is found by a single local search, or less local searches than threads.

As the left bottom graph of Figure 2 shows, the speed gain with additional threads in case of Shubert is countered by the NFEV and further decreased by the thread synchronization. An interesting feature is the higher relative speed with higher hardness levels, regardless of thread count. This is caused by the limit of the evaluation timing when applying hardness. Timing of low complexity function evaluations can be very inaccurate and constant overheads in execution exist, causing a non-linear relationship between NFEV and runtime. This effect evens out lower hardnesses and smaller NFEVs more. With a T1H0 configuration (1 thread, 0 hardness) we have an execution of 110 FEVs and 27 ms runtime. The same setup also executed with 1186 FEVs and 59 ms runtime which is 10 times the evaluations but only twice the runtime. This effect is almost negligible with H3 configurations. Unlike the Poolless version, the execution speed decreases with added threads, even with higher hardnesses. This is also caused by multiple factors interacting. The Poolless version on a single thread uses on average 16 local searches which means that 16 simultaneous local searches will have almost the same effect, pushing up the number of local searches with additional threads slightly. The poolless version uses



Figure 3: Relative runtimes on all test functions with 16 threads and hardness 3.

around 3000 FEVs with 16 threads that are almost entirely used in local searches. On the other hand the pooled version uses only 3 local searches on a single thread and over 3 it closely matches the number of threads. On 16 threads 1500 FEVs in 16 local searches are needed but 8000 FEVs are necessary in total. This shows that the addition of the sample pool both helped and worsened the optimizer for this particular type of function.

The top right graph of Figure 2 shows what we stated above; the pooled implementation erased the 2^1 multiplier in NFEV, it evened the Global and ParallelGlobal algorithms. Similar to the Poolless implementation we have close to linear speedup with additional threads with hardness 3 and significant speedups on lower hardness values. On this function optimizers need a lot of local searches, therefore ParallelGlobal managed to accelerate the process.

We deliberately chose *Shubert* and *Spikes* to showcase a good and bad scenario for the single thread and parallel optimizers as well. *Shubert* can be solved with few longer local searches, while *Spikes* needing only random sampling is the exact opposite. Figure 3 shows the overall picture on all of the tested functions.

On Figure 3 we show relative runtimes for the configuration of 16 threads and hardness 3 (T16H3) on every test function. Since the plot is logarithmic, 2^0 and values below mean similar and better results compared to Global. Error bars show the minimum and maximum data points from the averaged 100. On the functions which experienced slowdown either the lack of a sample pool or the intrinsic properties of ParallelGlobal prevented gains in speed. More than 50% of the functions with speedup were solved successfully, in these cases the NFEV limit had no effect.

5 Conclusion

We came to multiple important conclusions about the ParallelGlobal algorithm. The most needed change is the implementation of a distributed sample pool with sample sharing between threads. Having a set of probe points in the search space ensures that local searches only start from promising regions. This change moved the algorithm much closer to the NFEV values of Global. Many of our results show slowdown with ParallelGlobal, but huge improvements as hardness values increase, as we have seen on the *Spikes* function. To keep our run times manageable we kept the hardness value relatively low. By going up from the current millisecond order to the second or 10 second order in function evaluations we would have a clearer image on how much speedup can we achieve. This would still undershoot the evaluation time of many practical problems, however it would be sufficient for proper testing on distributed systems.

To achieve these improvements, first the addition of a distributed framework is needed. Both the sharing of probe samples and cluster information would rely on it. It is also a key for testing on computationally expensive problems.

Acknowledgments

This work was supported by the Hungarian Government under the grant number EFOP-3.6.1-16-2016-00008. The project has been supported by the European Union, cofunded by the European Social Fund, and by the János Bolyai Research Scholarship of the Hungarian Academy of Sciences.

References

- B. Bánhelyi, T. Csendes, B. Lévai, L. Pál, and D. Zombori. *The GLOBAL Optimization Algorithm*. Springer, 2018. https://doi.org/10.1007/ 978-3-030-02375-1.
- [2] B. Betró and F. Schoen. Optimal and suboptimal stopping rules for the multistart algorithm in global optimization. *Mathematical Programming*, 57:445–458, 1992. https://doi.org/ 10.1007/BF01581094.
- [3] C. G. E. Boender and A. H. G. Rinnooy Kan. On when to stop sampling for the maximum. *Journal of Global Optimization*, 1:331–340, 1991. https:// doi.org/10.1007/BF00130829.

- [4] C. G. E. Boender, A. H. G. Rinnooy Kan, G. Timmer, and L. Stougie. A stochastic method for global optimization. *Mathematical Programming*, 22:125–140, 1982. https://doi.org/10.1007/BF01581033.
- [5] T. Csendes, B. M. Garay, and B. Bánhelyi. A verified optimization technique to locate chaotic regions of Hénon systems. *Journal of Global Optimization*, 35:145–160, 2006. https://doi.org/10. 1007/s10898-005-1509-9.
- [6] T. Csendes, L. Pál, J. Sendin, and J. Banga. The global optimization method revisited. *Optimization Letters*, 2:445–454, 2008. https://doi.org/ 10.1007/s11590-007-0072-3.
- [7] A. Szenes, B. Bánhelyi, L. Zs. Szabó, G. Szabó, T. Csendes, and M. Csete. Improved emission of SiV diamond color centers embedded into concave plasmonic core-shell nanoresonators. *Scientific Reports*, 7:an:13845, 2017. https://doi.org/ 10.1038/s41598-017-14227-w.
- [8] I. Lagaris and I. Tsoulos. Stopping rules for box-constrained stochastic global optimization. In Applied Mathematics and Computation, 197:622– 632, 2008. https://doi.org/10.1016/j. amc.2007.08.001.
- [9] J. Sendín, J. Banga, and T. Csendes. Extensions of a multistart clustering algorithm for constrained global optimization problems. *Industrial & Engineering Chemistry Research*, 48:3014–3023, 2009. https: //doi.org/10.1021/ie800319m.
- [10] S. Surjanovic and D. Bingham. http://www. sfu.ca/~ssurjano/optimization.html.
- [11] A. A. Törn. A search clustering approach to global optimization. *Towards Global Optimization 2.*, pages 49–62, 1978.