

Preconditioned Spectral Clustering for Stochastic Block Partition Streaming Graph Challenge

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Abstract

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IEEE HPEC Graph Challenge

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Preconditioned Spectral Clustering for Stochastic Block Partition Streaming Graph Challenge

(Preliminary version at arXiv.)

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Abstract—Locally Optimal Block Preconditioned Conjugate Gradient (LOBPCG) is demonstrated to efficiently solve eigenvalue problems for graph Laplacians that appear in spectral clustering. For static graph partitioning, 10–20 iterations of LOBPCG without preconditioning result in ~10x error reduction, enough to achieve 100% correctness for all Challenge datasets with known truth partitions, e.g., for graphs with 5K/1M (50K/1M) Vertices/Edges in 2 (7) seconds, compared to over 5,000 (30,000) seconds needed by the baseline Python code. Our Python code 100% correctly determines 98 (160) clusters from the Challenge static graphs with 0.5M (2M) vertices in 270 (1,700) seconds using 10GB (50GB) of memory. Our single-precision MATLAB code calculates the same clusters at half time and memory. For streaming graph partitioning, LOBPCG is initiated with approximate eigenvectors of the graph Laplacian already computed for the previous graph, in many cases reducing 2-3 times the number of required LOBPCG iterations, compared to the static case. Our spectral clustering is generic, i.e. assuming nothing specific of the block model or streaming, used to generate the graphs for the Challenge, in contrast to the base code. Nevertheless, in 10-stage streaming comparison with the base code for the 5K graph, the quality of our clusters is similar or better starting at stage 4 (7) for emerging edging (snowballing) streaming, while the computing time is 100–1000 smaller.

I. INTRODUCTION

Spectral clustering is a classical method for grouping together relevant data points, while at the same time separating irrelevant data points. Spectral clustering is commonly formulated as a partitioning of a graph, with vertices of the graph being mapped with data points. The clustering is called “spectral” because its algorithms are based on spectral graph theory, i.e. spectral properties of matrices associated with the graph, such as graph adjacency and Laplacian matrices, and thus can be related to dimensionality reduction via the principal component analysis. Compared to other practical clustering techniques, spectral clustering is arguably well supported mathematically, mostly avoiding heuristic simplifications, typically needed in combinatorial optimization formulations of clustering to make computations tractable. Spectral clustering has been successful in a wide variety of applications, ranging from traditional resource allocation, image segmentation, and information retrieval, to more recent bio-informatics, providing meaningful results at reasonable costs.

The graph partitioning problem can be formulated in terms of spectral graph theory, e.g., using a spectral decomposition of a graph Laplacian matrix, obtained from a graph adjacency matrix with non-negative entries that represent positive graph edge weights describing similarities of graph vertices. Most commonly, a multi-way graph partitioning is obtained from approximated “low frequency eigenmodes,” i.e. eigenvectors corresponding to the smallest eigenvalues, of the graph Laplacian matrix. Alternatively and, in some cases, e.g., normalized cuts, equivalently, one can operate with a properly scaled graph adjacency matrix, turning it into a row-stochastic matrix that describes probabilities of a random walk on the graph, where the goal is to approximate the dominant eigenpairs.

The Fiedler vector, or a group of eigenvectors of the graph Laplacian corresponding to the left-most eigenvalues, are computed iteratively by solving the corresponding symmetric eigenvalue problem. Efficiency of iterative solvers is crucial for practical computations for large or real time streaming data. The need to deal with big data and the resulting humongous matrix eigenvalue problems in data sciences is not historically the first one. Computational mechanics and especially material sciences have long been sources of large scale eigenvalue problems, with the increasing needs outgrowing all advances in computing resources. For example, a decade ago two Gordon Bell Prize finalists at ACM/IEEE Conferences on Supercomputing in 2005 [1] and 2006 [2] implemented on Japan’s Earth Simulator—the number one supercomputer in the world at that time,—and successfully tested, for multi-billion size matrices, the Lanczos [3] and Locally Optimal Block Preconditioned Conjugate Gradient (LOBPCG) [4] methods.

The remainder of the paper is organized as follows. In §II, we briefly review, cf. [5], [6], traditional graph-based spectral clustering and cuts partitioning, discuss numerical issues of related large scale computations for Big Data spectral clustering, and describe our approach. Partition Challenge Datasets with Known Truth Partitions [7] suitable for our techniques are reviewed in §III. Our numerical results appear in §IV. We conclude in §IV that spectral clustering via LOBPCG is an efficient scalable technology for high-quality fast graph partitioning in the present era of Big Data.

II. APPROACH

A. Introduction to spectral clustering in a nutshell

Let entries of the matrix W be called *weights* and the matrix D be diagonal, made of row-sums of the matrix W . The matrix W may be viewed as a matrix of scores, which represent the similarity between of data points. Similarities are commonly determined from their counterparts, distances. The distance matrix is a matrix containing the distances, taken pairwise, of a set of data points. The general connection is that the similarity is small if the distance is large, and vice versa.

Commonly, the data clustering problem is formulated as a graph partition problem. The graph partition problem is defined on data represented in the form of a graph $G = (V, E)$, with n vertices V and m edges E such that it is possible to partition G into smaller components with specific properties. For instance, a k -way partition partitions the vertex set into k components. The similarity matrix W is provided as an input and consists of a quantitative assessment of the relative similarity of each pair of points in the dataset. In the framework of graph spectral partitioning, entries of the n -by- n matrix W are weights of the corresponding edges E , and the matrix W is called the *weighted graph adjacency* matrix.

Traditional mathematical definitions of graph partitioning are combinatorial and naturally fall under the category of NP-hard problems, solved using heuristics in practice. Data clustering via graph spectral partitioning, initiated in [8], [9], is a state-of-the-art tool, which is known to produce high quality clusters at reasonable costs.

In directed graphs, the weighted graph adjacency matrix W is not symmetric. For the purpose of spectral partitioning, which is based on eigenvalue decompositions of matrices associated with the graph, it is very convenient to deal with symmetric matrices, so the non-symmetric W is often symmetrized. The symmetrization we use is substituting $W + W'$ for W , where W' denoted the transpose of the matrix W and the sum $+$ may be logical if the graph has no weights, e.g., all non-zero entries in W are simply ones. In general, we assume that all the entries (weights) in W are non-negative real numbers and the sum is algebraic.

Let us introduce the graph Laplacian matrix $L = D - W$. The column-vector of ones is always an eigenvector of L corresponding to the zero eigenvalue. The symmetric matrix L has all non-negative eigenvalues, provided that all entries of the matrix W are nonnegative; cf. [10]. The actual number of major partitions is automatically determined in spectral clustering using a gap in the smallest eigenvalues of the graph Laplacian. The gap is calculated by comparing the increments in the eigenvalues to find the first significantly large increment. The number of eigenvalues located below the gap determines the number of major multi-way graph partitions/clusters. An absence of the gap indicates that no reliable multi-way graph partitioning is available. Multi-way block partition is computed from the matrix of approximate eigenvectors via QR factorization with column pivoting, shown in [11] to supplement or supersede the traditional k -means++.

B. Numerical challenges of spectral clustering

Our spectral clustering performs block partitioning of graphs using the Locally Optimal Block Preconditioned Conjugate Gradient (LOBPCG) method to iteratively approximate leading eigenvectors of the symmetric graph Laplacian for multi-way graph partitioning. The number of the eigenvectors should not subceed the number of anticipated partitions.

If further lower-level partitioning is desired, the multi-way clustering procedure described above can be repeated recursively to independently partition each of the already determined clusters, resulting in a hierarchical tree of block partitions. Our code, written for the IEEE HPEC Graph Challenge 2017 [7], does not have this feature implemented, performing only a single multi-way graph partitioning.

Both Lanczos and LOBPCG methods do not require storing a matrix of the eigenvalue problem in memory, but rather only need the results of multiplying the matrix by a given vector. Such a matrix-free characteristic of the methods makes them particularly useful for eigenvalue analysis problems of very large sizes, and results in good parallel scalability on multi-threaded computational platforms to large matrix sizes processed on many parallel processors.

Compared to Lanczos, LOBPCG is a block method, where several eigenvectors are computed simultaneously as in the classical subspace power method. Blocking is beneficial if the eigenvectors to be computed correspond to clustered eigenvalues, which is a typical scenario in multi-way spectral partitioning, where often a cluster of the smallest eigenvalues is separated by a gap from the rest of the spectrum. Blocking also allows taking advantage of high-level BLAS3-like libraries for matrix-matrix operations, which are typically included in CPU-optimized computational kernels.

LOBPCG may be optionally accelerated by preconditioning, if available, e.g., see [4], [12], [13], to speed up convergence, e.g., using Algebraic Multigrid Method (AMG) applied to a regularized graph Laplacian. The regularization is needed, since AMG attempts to mimic an action of a matrix inverse, while the original graph Laplacian is technically not invertible, always having the trivial constant eigenvector corresponding to the zero eigenvalue. AMG preconditioning increases the computational costs per iteration, but may reduce the number of required LOBPCG iterations. AMG preconditioning is known to perform extremely well for some classes of graphs, although may be inefficient for arbitrary graphs. Since preconditioning is optional in LOBPCG, it can be dynamically turned off or on, as well as AMG parameters may be tuned, depending on past performance in the case of streaming graph.

The open-source Python function of LOBPCG from SciPy is used for our numerical tests; cf., [14]. AMG and dense matrix factorizations, e.g., QR, are also performed by well-known open-source Python functions. Similar open-source LOBPCG and AMG functions are available in C with MPI and OpenMP parallel functionality, e.g., in hypre and PETSc/SLEPc [13], Trilinos/Anasazi [15] libraries, as well as GPU implementations in MAGMA [16] and NVIDIA nvGRAPH [17].

III. EXPERIMENTS

IEEE HPEC Streaming Graph Challenge Stochastic Block Partition seeks to identify optimal blocks (or clusters) in a graph. In static processing, given a large graph G the goal is to partition G . In stateful streaming, which is the focus of the streaming graph challenge, given an additional smaller graph g the goal is to partition $G + g$; see [7].

Taking advantage of the second author expertise in numerical solution of matrix eigenvalue problems, we have selected the graph partition challenge, for which spectral clustering is known in practice to produce high quality clusters at reasonable computational costs. The costs of spectral clustering are primarily determined by a choice of an eigenvalue solver. All eigenvalue solvers are by nature iterative, so one needs to minimize the costs per iteration as well the total number of iterations needed to achieve the required accuracy of clustering. The LOBPCG eigenvalue solver, that we have selected to use, only requires the result of single multiplication of the graph adjacency matrix by a vector (or a group of vectors that is called a multi-vector) per iteration, just as the classical power method.

For static graphs, the initial approximations for the eigenvectors of the graph Laplacian in LOBPCG are chosen randomly—every component of every eigenvector is Gaussian or uniformly distributed on $[-1,1]$. Such randomization helps LOBPCG to avoid local stationary points in the iterative process of convergence to the leading eigenvectors. Streaming graphs are treated via warm-starts of LOBPCG, where the approximate eigenvectors already computed for the previous graph in the stream serve as high-quality initial approximations in LOBPCG for the graph Laplacian of the current graph. Such warm-starts of LOBPCG may significantly reduce the number of iterations of LOBPCG, compared to the randomized initialization for the static case, if the streaming graph is sampled often enough. To enable possible appearance of additional partitions of the streaming graph one should choose the starting number of the eigenvectors to be computed large enough and keep it, or determine the number of computed eigenvectors dynamically, always slightly exceeding (for the gap calculation) the expected number of partitions.

Streaming graphs with dynamically changing numbers of vertices, like in the snowball example, can also be efficiently processed by LOBPCG with warm-starts, if a mapping is known between the sets of old and new vertices. In the snowball example, the old vertices are always numbered first and in the same order in a subset of the new vertices, thus for warm-starts we put the previously computed eigenvectors in the top block of the initial approximate eigenvectors for the current graph. Since the set of vertices in the snowball example is growing, warm-starts require filling the missing entries in the bottom block of the initial approximate eigenvectors for the current graph. One can fill in the missing entries by random or use interpolation of the already available values in the old vertices, e.g., by propagating the values using the graph connectivity. In our tests, we use the random fill-in.

We have limited our testing to Partition Challenge Datasets with Known Truth Partitions. In terms of the number of vertices of the graphs, our MATLAB, Python, and C codes partition the Challenge static 5K graph 100% correctly in a second, already making reliable timing difficult, so 5K is the smallest size we have tested. Our Python code runs out of 128 GB memory in the case of 5M vertices with 221 partitions, so our largest tested Challenge graph is with 2M vertices.

There are public eigensolvers in C with MPI, allowing well-scalable parallel distributed-memory solution of eigenvalue problems, e.g., LOBPCG in hypre and PETSc/SLEPc [13], Trilinos/Anasazi [15], and MAGMA [16]. We have performed preliminary tests with LOBPCG in hypre and PETSc/SLEPc/BLOPEX on a single node, but observe no dramatic increase of performance, compared to our Python and MATLAB codes, so do not report the corresponding results in the present work. Our explanation is that, to our knowledge, the present versions of LOBPCG in hypre and SLEPc/BLOPEX implement the distributed column-matrix multi-vector X only rudimentarily, as a collection of distributed single vectors, which does not allow utilizing highly efficient matrix-matrix BLAS-3 type libraries. In contrast, PETSc/SLEPc, Trilinos/Anasazi, and MAGMA versions of LOBPCG pay special attention to efficient implementation of distributed multi-vectors and thus are expected to perform well both in shared and distributed memory environments.

Our Python and MATLAB codes do not use MPI, so all our tests are on a single node. However, the BLAS and LAPACK-type functions in Python and MATLAB are multi-threaded and most expensive operations in LOBPCG are matrix-matrix BLAS-3 type, so multiple cores are being used.

We test matrix-free versions of our codes, where the original non-symmetric adjacency matrix A is read from the given file and stored in binary sparse matrix format, and where the required by LOBPCG multiplication of the graph Laplacian L by a column-matrix (block of vectors) X is performed by a function call, e.g., $LXfun = @(X)diagL.*X - A.*X - (X'.*A)'$ in MATLAB, wherein the vector $diagL$ contains pre-computed diagonal entries of L . AMG commonly needs the matrix L of the graph Laplacian being explicitly available, however. We have found that our matrix-free implementations in Python and MATLAB lead to no decrease in computing time, although saves memory for matrix storage.

The Python AMG has not led to acceleration in our tests, and the corresponding results are not shown. We have also tested LOBPCG in hypre and PETSc/SLEPc with hypre algebraic multigrid BoomerAMG, but observed no advantages, so we report no results here. Our explanation is that LOBPCG has been able to determine 100% correct partition typically after a relatively small, 10–20, number of iterations, even without AMG. The extra costs of constructing and applying AMG preconditioning that we have tested are significant, due to a large, relative to that in typical AMG use for partial differential equations, vertex degrees. Preconditioning for graph Laplacians is a competitive research area, but we have limited testing to MPI software available via PETSc.

TABLE I

TYPICAL PYTHON TIMING IN SEC FOR 100% CORRECT PARTITION OF STATIC GRAPHS FROM THE CHALLENGE DATASETS WITH KNOWN TRUTH

$ V / E $	5K/.1M	20K/.4M	50K/1M	.5M/10M	2M/41M
# Clusters	19	32	44	98	160
LOBPCG	<1	2	7	270	1700
Base	400	5100	30000	N/A	N/A

IV. RESULTS

We have tested our MATLAB, Python, and C codes on several platforms, ranging from MS Windows and MAC laptops to r4.16xlarge AWS EC2 instances. Typical timing in seconds for 100% correct partition of static graphs in Table I is for a single node with 20 cores of Intel Xeon CPU E5-2660 v3 2.60GHz and 128 GB DDR4 RAM. We have not attempted to run the base Python code for graphs with over 50K vertices.

Checking scalability as the size of the graph increases in Table I, we see that the timing grows at least linearly with the product of the number of edges $m = |E|$ and the number of clusters, we denote by k . We remind the reader that we simultaneously compute l approximate eigenvectors in LOBPCG and keep l slightly larger than the expected number k of the clusters. LOBPCG performs linear algebraic operations with multi-vectors (n -by- l matrices), at the cost proportional to $n \cdot l \approx n \cdot k$. In single-precision MATLAB tests, not reported here, but where we get more stable timing measurement for graphs with 20K and smaller vertices, for 10x growth from the graph size 5K/.1M Vertices/Edges to 50K/1M Vertices/Edges at the same time increases 2.5x the number of clusters from 19 to 44, resulting in approximately 25x increase in computation time from .3 sec to 7 sec. In Table I, 10x growth from the graph size 50K/1M Vertices/Edges to .5/10M Vertices/Edges at the same time increases 2.2x the number of clusters k from 44 to 98, resulting in approximately 40x increase in computation time from 7 sec to 270 sec, so it appears that the growth may be quadratic in k .

Indeed, LOBPCG also computes Gram matrices for multi-vectors, which has the computational cost proportional to $n \cdot l^2$. When the number $k \leq l$ of the clusters grows, this quadratic term in the costs may start dominating. However, we observe in Table I that 4x growth from the graph size .5M/10M Vertices/Edges to 2M/40M Vertices/Edges at the same time increases 1.6x the number of clusters k from 98 to 160, but resulting in only 6.3x increase in computation time from 270 sec to 1700 sec, which is linear in $n \cdot k$. This effect may be explained by faster convergence for larger k and efficient soft locking [18] of already converged eigenvectors in LOBPCG.

The main memory usage in LOBPCG is for 6 multi-vectors—matrices of the size n -by- l , in addition to whatever memory is needed to store the adjacency matrix A or its equivalent, that is required to perform the multiplication of a multi-vector by the graph Laplacian. Simultaneous computing of $l = 162$ eigenvectors for the graph with 2M/40M Vertices/Edges requires approximately 50 (25) GB of RAM in double (single) precision in our Python (MATLAB) codes.

To save memory, LOBPCG can also perform hard-locking, i.e. compute eigenvectors one-by-one or block-by-block, in the constrained subspace that is complementary to all previously computed eigenvectors. Hard-locking is implemented in all LOBPCG versions, and is easy to use, but may lead to slower LOBPCG convergence. Even more radical memory saving approach would be recursive spectral bisection, which however would likely decrease both the convergence speed and the quality of partition. The Challenge graphs are small enough not to have forced the issue, allowing multi-way partitioning simply using the full block-size in LOBPCG without hard-locking, except for the largest graph with 5M vertices, when our code runs out of memory.

Our main Python and MATLAB codes are very short, but call the LOBPCG function and a few standard functions for matrix computations, e.g., available in LAPACK.

Accuracy of partitions for the streaming Partition Challenge Datasets with Known Truth Partitions is displayed using optimal partition matching (PM), pairwise recall (PR), and pairwise precision (PP). We report separately the results of streaming with random (R) and warm-start (W) initialization.

Our spectral clustering is generic, i.e., based entirely on the graph adjacency matrix, not making any assumptions specific to the block model, used to generate the graphs for the Challenge, in contrast to the baseline code. Unsurprisingly, PM and PP values for our partitions may at initial stages of graph streaming be small, relative to those for the base code, for small-size graphs, since the spectral gap may determine the number of clusters different from k . We report the correctness only at stages 5 – 10 of the streaming process, except for 5K and 2M cases, where we provide the complete data.

The timing is reported in seconds in all tables. Using the warm-start (W) in LOBPCG compared to random (R) initialization may not only speeds up LOBPCG convergence, but has also typically positive effect on correctness of the partition, especially in the case of emerging edges.

Partitioning streaming graphs with snowballing effects brings new challenges, compared to the case of emerging edges. Since new vertices emerge in the streaming, we have to come up with the warm-start procedure, which gives us the values to initialize eigenvector components corresponding to the previously missing vertices for our vertex-based graph Laplacian spectral clustering.

We resort to the trivial scenario, where the missing values are just chosen randomly, while the previously computed values are reused wherever available. Such a warm-start is somewhat beneficial in some tests, compared to random initialization of all components of approximate eigenvectors, but not as good as for emerging edges. We conjecture that better results might be obtained via graph-based signal reconstruction techniques, such as in [19], that interpolate a given signal on some vertices of a graph to all the vertices, using low-pass graph based filters.

We finally note that due to random initialization numerical results somewhat vary when tests repeated even on the same hardware. The presented results are typical, in our experience.

TABLE II
5K EMERGING (TOP) AND SNOWBALL (BOTTOM) BASE VS. LOBPCG

V	Base				LOBPCG warm-start			
	sec	PM	PR	PP	sec	PM	PR	PP
1	507	.088	1	.056	.5	.14	.21	.08
2	617	.941	.97	.895	.5	.09	.99	.06
3	460	.996	.992	.993	.5	.09	.99	.06
4	447	.919	.868	.999	.7	.97	.98	.96
5	439	1	1	1	.7	.99	.98	1
6	446	.919	.869	1	1.1	.97	.99	.96
7	442	.926	.871	1	.7	1	1	1
8	432	1	1	1	.8	1	1	1
9	415	1	1	1	1.1	1	1	1
10	409	.921	.869	1	1.4	1	1	1
1	22	.550	.382	.656	.2	.34	.999	.14
2	52	.915	.751	.981	.2	.25	.973	.08
3	80	.999	.999	.999	.2	.93	.929	.99
4	113	1	1	1	.4	.13	.988	.06
5	146	1	1	1	.3	.27	.985	.08
6	190	1	1	1	.4	.26	.999	.08
7	244	1	1	1	.4	1	1	1
8	298	1	1	1	1.3	1	1	1
9	366	1	1	1	1	1	1	1
10	416	1	1	1	1.4	1	1	1

TABLE III
2M EMERGING (TOP) AND SNOWBALL (BOTTOM) LOBPCG RANDOM VS. WARM-START

#	secR	secW	PMR	PMW	PRR	PRW	PPR	PPW
1	850	800	.016	.016	.008	.344	.008	.007
2	1200	1000	.014	.013	.354	.662	.007	.007
3	2100	1600	.019	.013	.784	.916	.007	.007
4	3300	4700	.013	.013	1	1	.007	.007
5	3300	2600	.013	.013	1	1	.007	.007
6	2800	2800	.013	.013	1	1	.007	.007
7	3000	1500	.013	.964	1	.993	.007	.943
8	2600	1200	1	.992	1	.999	1	.991
9	3000	800	1	1	1	1	1	1
10	3800	1600	1	1	1	1	1	1
1	440	420	.08	.08	.998	.998	.014	.014
2	1020	960	.037	.037	1	1	.008	.008
3	1110	1400	.024	.083	1	.794	.007	.012
4	1450	1570	.02	.02	.999	.98	.007	.007
5	1660	2000	.015	.015	.999	.999	.007	.007
6	2260	2000	.037	.838	.993	.941	.007	.669
7	1980	720	.036	.953	.999	.995	.007	.912
8	1840	1140	1	.998	1	1	1	.998
9	2400	710	1	1	1	1	1	1
10	3800	3200	1	1	1	1	1	1

V. CONCLUSION

We review algorithms and software for eigenvalue problems, focusing on LOBPCG for spectral clustering and describing our spectral multi-way graph partitioning implemented in Python, MATLAB and C. Our tests for all static graphs in the Challenge demonstrate 100% correct partition, even though our spectral clustering approach is general, not tailored for the stochastic block model used to generate the graphs. Our Python code is at least 100–1000 times faster for all tested graphs with 5K and more vertices compared to the baseline Python dense serial implementation of the reference method. Potential next steps include testing SLEPc, Trilinos/Anasazi, MAGMA, and CUDA versions of LOBPCG in shared and distributed memory environments for practical graph partitioning.

REFERENCES

- [1] S. Yamada, T. Imamura, and M. Machida, “16.447 tflops and 159-billion-dimensional exact-diagonalization for trapped fermion-hubbard model on the earth simulator,” in *Supercomputing, 2005. Proceedings of the ACM/IEEE SC 2005 Conference*, Nov 2005, pp. 44–44, doi:10.1109/SC.2005.1.
- [2] S. Yamada, T. Imamura, T. Kano, and M. Machida, “High-performance computing for exact numerical approaches to quantum many-body problems on the earth simulator,” in *Proceedings of the 2006 ACM/IEEE Conference on Supercomputing*, ser. SC '06. New York, NY, USA: ACM, 2006, doi:10.1145/1188455.1188504.
- [3] C. Lanczos, “An iterative method for the solution of the eigenvalue problem of linear differential and integral,” *J. Res. Natl Bur. Std.*, vol. 45, pp. 225–282, 1950, doi:10.6028/jres.045.026.
- [4] A. Knyazev, “Toward the optimal preconditioned eigensolver: locally optimal block preconditioned conjugate gradient method,” *SIAM J. Scientific Computing*, vol. 23, no. 2, pp. 517–541, 2001, doi:10.1561/06000000020.
- [5] U. Luxburg, “A tutorial on spectral clustering,” *Statistics and Computing*, vol. 17, no. 4, pp. 395–416, 2007, doi:10.1007/s11222-007-9033-z. [Online]. Available: <http://dx.doi.org/10.1007/s11222-007-9033-z>
- [6] J. Liu and J. Han, “Spectral clustering,” in *Data Clustering: Algorithms and Applications*, C. Aggarwal and C. Reddy, Eds. Chapman Hall/CRC Press, 2013, <http://www.crcnetbase.com/doi/pdf/10.1201/b15410-9>.
- [7] E. Kao, V. Gadepally, M. Hurley, M. Jones, J. Kepner, S. Mohindra, P. Monticciolo, A. Reuther, S. Samsi, W. Song, D. Staheli, and S. Smith, “Streaming Graph Challenge: Stochastic Block Partition,” in *IEEE HPEC*, 2017, <http://graphchallenge.mit.edu/challenges>.
- [8] M. Fiedler, “Algebraic connectivity of graphs,” *Czechoslovak mathematical journal*, vol. 23, no. 2, pp. 298–305, 1973, <http://dml.cz/handle/10338.dmlcz/101168>.
- [9] —, “A property of eigenvectors of nonnegative symmetric matrices and its application to graph theory,” *Czechoslovak Mathematical Journal*, vol. 25, no. 4, pp. 619–633, 1975, <http://hdl.handle.net/10338.dmlcz/101357>.
- [10] A. V. Knyazev, “Signed Laplacian for spectral clustering revisited,” *ArXiv e-prints*, Jan. 2017, <https://arxiv.org/abs/1701.01394>.
- [11] A. Damlé, V. Minden, and L. Ying, “Robust and efficient multi-way spectral clustering,” *ArXiv e-prints*, Sep. 2016. [Online]. Available: <http://adsabs.harvard.edu/abs/2016arXiv160908251D>
- [12] A. V. Knyazev, “Modern preconditioned eigensolvers for spectral image segmentation and graph bisection,” in *Proceedings of the workshop Clustering Large Data Sets; Third IEEE International Conference on Data Mining (ICDM 2003)*, Boley, Dhillon, Ghosh, and Kogan, Eds. Melbourne, Florida: IEEE Computer Society, 2003, pp. 59–62, <http://math.ucdenver.edu/~aknyazev/research/conf/ICDM03.pdf>.
- [13] A. V. Knyazev, M. E. Argentati, I. Lashuk, and E. E. Ovtchinnikov, “Block locally optimal preconditioned eigenvalue solvers (blopex) in hypre and petsc,” *SIAM J. Scientific Computing*, vol. 29, no. 5, pp. 2224–2239, 2007, <http://dx.doi.org/10.1137/060661624>.
- [14] J. McQueen, M. Meila, J. VanderPlas, and Z. Zhang, “megaman: Manifold learning with millions of points,” *CoRR*, vol. abs/1603.02763, 2016. [Online]. Available: <http://arxiv.org/abs/1603.02763>
- [15] E. Boman, K. Devine, R. Lehoucq, N. Slattengren, and H. Thornquist, “Installing the anasazi eigensolver package with application to some graph eigenvalue problems,” Tech. Report SAND2014-16610, Sandia National Labs, Tech. Rep., 2014, <http://trilinos.org/wordpress/wp-content/uploads/2014/08/anasazi-ug-public.pdf>.
- [16] H. Anzt, S. Tomov, and J. Dongarra, “On the performance and energy efficiency of sparse linear algebra on GPUs,” *The International Journal of High Performance Computing Applications*, pp. 1–16, 2016, doi:10.1177/1094342016672081.
- [17] M. Naumov, “Fast spectral graph partitioning on gpus,” Technical notes, NVIDIA Parallel Forall, Tech. Rep., 2016. [Online]. Available: <https://devblogs.nvidia.com/parallelforall/fast-spectral-graph-partitioning-gpus/>
- [18] A. Knyazev, “Hard and soft locking in iterative methods for symmetric eigenvalue problems,” in *Presentation at the Eighth Copper Mountain Conference on Iterative Methods*, 2004, http://math.ucdenver.edu/~aknyazev/research/conf/cm04_soft_locking/cm04.pdf.
- [19] A. Knyazev and A. Malyshev, “Signal reconstruction via operator guiding,” *ArXiv e-prints*, May 2017, <https://arxiv.org/abs/1705.03493>.

TABLE IV
EMERGING EDGES STAGES 5–10 LOBPCG PYTHON

Stage 5					
V	5K	20K	50K	.5M	2M
sec R	.8	5	14	443	3300
sec W	.7	3	4	373	2600
PM R	.99	.965	.892	.021	.013
PM W	.99	.98	.903	.021	.013
PR R	.979	.988	.952	.999	1
PR W	.98	.99	.971	.998	1
PP R	1.0	.952	.822	.011	.007
PP W	1.0	.974	.848	.011	.007
Stage 6					
V	5K	20K	50K	.5M	2M
sec R	.7	4	15	520	280
sec W	1.1	1.3	4	290	2800
PM R	.97	.999	.991	.039	.013
PM W	.97	.983	.983	.917	.013
PR R	.988	.997	.997	.998	1
PR W	.988	.998	.996	.979	1
PP R	.957	1.0	.987	.012	.007
PP W	.957	.984	.968	.85	.007
Stage 7					
V	5K	20K	50K	.5M	2M
sec R	.9	4.6	10	380	3000
sec W	.7	1.4	7	280	1500
PM R	1	1	.992	.039	.013
PM W	1	1	.992	.987	.964
PR R	1	1	.997	1.0	1
PR W	1	1	.997	.999	.993
PP R	1	1	.987	.012	.007
PP W	1	1	.987	.982	.943
Stage 8					
V	5K	20K	50K	.5M	2M
sec R	.9	3	10	360	2600
sec W	.8	4	4	160	1200
PM R	1	1	.992	.997	1
PM W	1	1	.992	1	.992
PR R	1	1	.997	.999	1
PR W	1	1	.997	1	.999
PP R	1	1	.987	.995	1
PP W	1	1	.987	1	.991
Stage 9					
V	5K	20K	50K	.5M	2M
sec R	1	4.5	10	480	3000
sec W	1	1.4	6	260	800
PM R	1	1	1	1	1
PM W	1	1	1	1	1
PR R	1	1	1	1	1
PR W	1	1	1	1	1
PP R	1	1	1	1	1
PP W	1	1	1	1	1
Stage 10					
V	5K	20K	50K	.5M	2M
sec R	1.7	4.8	16	800	3800
sec W	1.4	5.6	20	600	1600
PM R	1	1	1	1	1
PM W	1	1	1	1	1
PR R	1	1	1	1	1
PR W	1	1	1	1	1
PP R	1	1	1	1	1
PP W	1	1	1	1	1

TABLE V
SNOWBALL STAGES 5–10 LOBPCG PYTHON

Stage 5					
V	5K	20K	50K	.5M	2M
sec R	.4	1.3	5.5	280	1660
sec W	.3	1.2	3.7	200	2000
PM R	.268	.963	.337	.02	.015
PM W	.268	.997	.965	.02	.015
PR R	.985	.989	.975	.999	.999
PR W	.985	.993	.989	.999	.999
PP R	.082	.933	.049	.011	.007
PP W	.083	1	.946	.011	.007
Stage 6					
V	5K	20K	50K	.5M	2M
sec R	.5	1.6	5.7	310	2260
sec W	.4	.8	4	110	2000
PM R	.262	.998	.991	.038	.37
PM W	.262	.998	.979	.946	.838
PR R	.999	.996	.996	.999	.993
PR W	.999	.997	.991	.99	.941
PP R	.082	1	.986	.012	.007
PP W	.082	1	.967	.908	.669
Stage 7					
V	5K	20K	50K	.5M	2M
sec R	.7	2	7.7	270	1980
sec W	.4	1.3	3	200	720
PM R	1	.998	1	.038	.036
PM W	1	.999	.992	.992	.953
PR R	1	.996	.999	.1	.999
PR W	1	.999	.997	.999	.995
PP R	1	1	1	.012	.007
PP W	1	1	.987	.988	.912
Stage 8					
V	5K	20K	50K	.5M	2M
sec R	.9	2.3	8.9	320	1840
sec W	1.3	2	4.5	170	1140
PM R	1	1	1	.997	1
PM W	1	1	1	.997	.998
PR R	1	1	1	.999	1
PR W	1	1	1	.999	1
PP R	1	1	1	.996	1
PP W	1	1	1	.996	.998
Stage 9					
V	5K	20K	50K	.5M	2M
sec R	1.2	2.9	9.8	340	2400
sec W	1	5.5	6.2	380	710
PM R	1	1	1	.997	1
PM W	1	1	1	.997	1
PR R	1	1	1	.999	1
PR W	1	1	1	.999	1
PP R	1	1	1	.996	1
PP W	1	1	1	.996	1
Stage 10					
V	5K	20K	50K	.5M	2M
sec R	1.4	7	18	670	3800
sec W	1.4	5	19	550	3200
PM R	1	1	1	1	1
PM W	1	1	1	1	1
PR R	1	1	1	1	1
PR W	1	1	1	1	1
PP R	1	1	1	1	1
PP W	1	1	1	1	1