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科学研究費助成事業（科学研究費補助金）研究成果報告書

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研究課題名（和文）幾何計算のためのソフトウェア開発：理論的基礎，実装とその応用
研究課題名（英文）Polyhedral computation, discrete optimization and quantum information
研究代表者
エイビス・デイビッド（AVIS David）
京都大学・情報学研究科・教授
研究者番号：90584110

研究成果の概要（和文）：
当該研究の目的は京都大学における幾何計算研究拠点の設立であり、現在その目的は達成されている。ここでは、主として３つの課題、多面体計算、離散最適化、量子情報について取り組んだ。これらの課題の共通テーマは高次元幾何であり、とりわけ多面体とそれに関わる凸体の研究である。また、ここでは、質の高い理論結果を生み出すとともに、それらの結果の工学・科学分野における広い利用を可能にするソフトウェアの開発も行っている。

研究成果の概要（英文）：The purpose of this grant was to provide funds for the new Geometric Computation Laboratory at Kyoto University which I have now established. This laboratory is concerned primarily with the following three research topics: polyhedral computation, discrete optimization and quantum information. The common theme linking these three topics is high dimensional geometry, and in particular, the study of polyhedra and related convex bodies. In addition to high quality theoretical results, the Geometric Computation Laboratory has been developing software that allows the results to be used widely in the engineering and scientific community.

交付決定額

（金額単位：円）

	直接経費	間接経費	合　計
2010 年度	1,260,000	378,000	1,638,000
2011 年度	1,160,000	348,000	1,508,000
年度			
年度			
年度			
総　計	2,420,000	726,000	3,146,000

研究分野：総合領域
科研費の分科・細目：情報学・情報学基礎
キーワード：計算幾何学，離散幾何学，アルゴリズム理論，量子情報

１．研究開始当初の背景　A vast array of important practical optimization problems can be modelled as high dimensional geometric problems. By high dimensional problems, we mean those where there is no fixed limit on the number of variables involved. Compared to low, fixed dimensional problems, high dimensional problems have the greatest potential for applications in many areas of engineering and science. Hence there is tremendous importance in designing and implementing software for this kind of problem. Due to the complexity of high dimensional geometric problems, we mainly focus on the most structured class of objects, convex bodies, and in particular polyhedra. Even here the inherent complexity is enormous, and

some basic computational problems regarding convex polyhedra are still unanswered. Important recent theoretical breakthroughs have enabled useful software to be developed that has wide application.

In the 1980s the field of Computational Geometry was developed with the goal of providing efficient methods for solving geometric problems on computers. While the techniques were very successful for problems in two or three dimensions, such as graphics, motion planning, etc. they did not scale well to higher dimensions. From the 1990s new methods started to be developed based on tools from Optimization, however the computational effort required to solve practical problems was enormous. Now however, with the availability of large scale multiprocessing hardware at reasonable prices, a vast improvement in what can be achieved computationally will occur. However many existing methods will not adapt well to this highly parallel architecture, and new algorithms and techniques will be required. This is the motivation for our research.

２．研究の目的 An important objective of our lab is to fully incorporate new theoretical insights into efficient and easy to use software for wide distribution. This is an essential point, as the sophistication of the underlying theory makes it virtually impossible to be implemented by someone not thoroughly familiar with it. One area of application that we were particularly concerned with is discrete optimization because of the tremendous practical application of results in this area in for society.

Although polyhedral methods have become an important tool in many areas of research in engineering and science, there is relatively little readily available software for the general researcher that exploits massive parallel architecture. My first goal was therefore to expand the tools that are able to harness the computational power available to the general researcher. The lrslib library package that uses reverse search was the ideal starting point for this project. Although special purpose parallel processing implementations have appeared in the past, these were not generally available or easily used. New features of the library were also implemented.

An important research topic on polyhedra relates to the complexity of linear programming. The search for a strongly polynomial time algorithm is surely the most important open problem in this area. My second goal is to study so-called history based rules for the simplex method to see if they will yield such an algorithm.

Another particularly important area of application of polyhedral techniques is in quantum information, where the power of ordinary communication can be modeled as convex polyhedra. More complicated convex sets model the power of quantum communication, and the study of these sets is at the heart of studying the limits of quantum theory when applied to this domain. My third goal was to extend our knowledge of the limits of quantum communication by using knowledge of the associated convex sets.

３．研究の方法 The research consisted of several subprojects in major research areas that spanned the two year grant period: history based pivot rules, ground metric learning, directed cuts and open pit mining, PageRank optimization, quantum information and a parallelization subproject for the lrs vertex enumeration code.
The schedule of research was as follows.
FY2011:
(1) Improved multicore version of the lrs vertex enumeration code
(2) Study of Zadeh’s pivot rules on hypercubes.
(3) Directed cut polyhedra
(4) Quantum information
FY2012:
(1)Multicore redundancy checking and new Fourier-Motzkin elimination program for lrslib
(2) Leggett-Garg inequalities
(3) Study of history based pivot rules for linear programming.
(4) Page Rank games

The Geometric Computation Lab received a series of high profile visits from established foreign researchers such as: K. Fukuda (ETH), S. Langerman (Bruxelles), I. Barany (Budapest), D. Rappaport (Queens), and L. Devroye (McGill). T. Deering, a graduate student from McGill spent an internship period at Kyoto University.

４．研究成果
(1) Study of Zadeh’s pivot rules on hypercubes
Klee and Minty showed that Dantzig’s pivot rule for the simplex method requires exponential time in the worst case. This analysis was extended to most other known pivot rules. However a family of history based pivot rules, introduced by Zadeh had defied analysis until Friedmann’s breakthrough in 2010 when he showed a

sub-exponential lower bound for the least entered rule. Aoshima, Deering, Matsumoto, Moriyama and I completed a paper on a systematic study of these pivot rules on abstract hypercubes. This will be published in Discrete Applied Mathematics.

(2) Ground Metric Learning

Transportation distances have been used for more than a decade now in machine learning to compare histograms of features. They have one parameter: the ground metric, which can be any metric between the features themselves. As is the case for all parameterized distances, transportation distances can only prove useful in practice when this parameter is carefully chosen. To date, the only option available to practitioners to set the ground metric parameter was to rely on a priori knowledge of the features, which limited considerably the scope of application of transportation distances. Cuturi and I proposed to lift this limitation and considered instead algorithms that can learn the ground metric using only a training set of labeled histograms. We called this approach ground metric learning. We formulated the problem of learning the ground metric as the minimization of the difference of two polyhedral convex functions over a convex set of distance matrices. We gave promising experimental results on binary classification tasks using GIST descriptors of images taken in the Caltech-256 set. We wrote a paper on this that is submitted to the Journal of Machine Learning, and was presented at the NIPS conference as a poster.

(3) Directed cuts and open pit mining

This application area project involved the geometric computational approach to solving practical open pit mining problems. To minimize mine costs, models have been made that involve finding directed cuts in a network. Conor Meagher (McGill) and I studied the related directed cut polyhedra and found classes of facets of these polyhedra that yield strong cutting planes. We presented this work at several international conferences and wrote a paper on this that is now being revised for publication.

(4) PageRank optimization

J. Hopcroft and D. Sheldon originally introduced network reputation games to investigate the self-interested behavior of web authors who want to maximize their PageRank on a directed web graph by choosing their outlinks in a game theoretic manner. They give best response strategies for each player and characterize properties of web graphs which are Nash equilibria. Iwama, Paku and I considered three different models for PageRank games on undirected graphs such as certain social networks. In undirected graphs players may delete links at will, but typically cannot add links without the other player's permission.

In the ED model players are free to delete any of their bidirectional links but may not add links.

We studied the problem of determining whether the given graph represents a Nash equilibrium or not in the ED model. We gave a quadratic time algorithm for a tree, and a parametric time algorithm for general graphs, depending on the maximum vertex degree in any biconnected component of the graph.

In the ECD model players are free to delete any biderctional links and add any directed links, since this addition can be done unilaterally. For this model we gave a cubic time algorithm for verifying Nash equilibria in trees.

Finally, in the EAD model we allowed a node to make arbitrary deletions and the addition of a single bidirectional link if it would increase the page rank of the other player also. In this model we give a parametric algorithm for verifying Nash equilibria in general graphs and characterize so called alpha-insensitive Nash Equilibria. We also give a result showing a large class of graphs where there is an edge addition that causes the PageRank of both of its endpoints to increase.

We presented this at ISAAC'12 and have prepared a full paper for submission to a refereed journal.

(5) Leggett-Garg inequalities

The Bell and Leggett-Garg tests offer operational ways to demonstrate that non-classical behavior manifests itself in quantum systems, and experimentalists have implemented these protocols to show that classical worldviews such as local realism and macrorealism are false, respectively. Previous theoretical research has exposed important connections between more general Bell inequalities and polyhedral combinatorics. Hayden, Wilde and I showed that general Leggett-Garg inequalities are closely related to the cut polytope of the complete graph, a geometric object well-studied in combinatorics. Building on that connection, we gave a family of Leggett-Garg inequalities that are not trivial combinations of the most basic Leggett-Garg inequalities. We then showed that violations of macrorealism can occur in surprising ways, by giving an example of a quantum system that violates the new "pentagon" Leggett-Garg inequality but does not violate any of the basic "triangle" Leggett-Garg inequalities.

(6) Multicore version of the lrs vertex enumeration code

We have finished a preliminary version of this program that has been tested on parallel hardware with 4 processors. Using the start-up grant we have purchased a 12 core machine to give a more powerful platform to verify this software prior to distribution.

The major feature of this implementation is that additional cores are utilized as they become available without user intervention.

５．主な発表論文等

（研究代表者、研究分担者及び連携研究者には下線）

〔雑誌論文〕（計 2 件）

①Y. Aoshima, D. Avis, T. Deering, Y. Matsumoto and S. Moriyama "On the Existence of Hamiltonian Paths for History Based Pivot Rules on Acyclic Unique Sink Orientations of Hypercubes," Discrete Applied Mathematics, accepted for publication, 2012.

② D. Avis, P. Hayden and M. Wilde "Leggett-Garg Inequalities and the Geometry of the Cut Polytope," Physical Review A, 2010.

〔学会発表〕（計 15 件）

① D. Avis, K. Iwama, D. Paku, “Verifying Nash Equilibria in PageRank Games on Undirected Web Graphs,” ISAAC 2011, December 2011

② D. Avis, “The Directed Cut Cone and Polytope with Mining Applications,” Conference on Discrete Geometry and Optimization, invited lecture, September 20, 2011, Fields Institute, University of Toronto

③ Y. Aoshima, D. Avis, T. Deering, Y. Matsumoto and S. Moriyama, “Enumerating Hamiltonian Paths on Acyclic USO Cube with History Based Pivot Rules,”AAAC2011, April 16, 2011, National Tsing Hua University, Taiwan.

④ D. Avis, “History Based Pivot Rules for Acyclic USOs on Hypercubes,” Efficiency of the Simplex Method: Quo Vadis the Hirsch Conjecture, invited lecture, January 19, 2011, IPAM, UCLA

⑤ D. Avis, "Those Ubiquitous Cut Polyhedra", Paul Erdos Memorial Lecture, 21st CCCG, Winnipeg, August 2010

⑥ D. Avis, "Recollections on the Discovery of the Reverse Search Technique," LA Symposium, 55(2010)14-16

⑦ D. Avis and C. Meagher, "Structural Properties of the Directed Cut Polytope," Canadian Math Society Summer Meeting, Fredericton, June 2010 14-16

〔その他〕

ホームページ等

http://www.i.kyoto-u.ac.jp/~avis

６．研究組織

(1)研究代表者

エイビス・デイビッド（AVIS David）

京都大学・情報学研究科・教授

研究者番号：90584110

(2)研究分担者

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研究者番号：

(3)連携研究者

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研究者番号：