

科学研究費助成事業 研究成果報告書

平成 28 年 6 月 21 日現在

機関番号：14301

研究種目：基盤研究(B) (一般)

研究期間：2012～2015

課題番号：24300002

研究課題名(和文)幾何計算アプローチによる計算困難な最適化問題の求解：理論的基盤と実装

研究課題名(英文)Geometric computational approach to solving hard optimization problems: theory and implementation

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交付決定額(研究期間全体)：(直接経費) 11,700,000円

研究成果の概要(和文)：本研究計画の目的は、申請者が2010年に設立した幾何計算研究室の研究目的を遂行することである。理工学の分野で高いインパクトを与えるものの、これまで計算困難であった問題を解く革新的なアルゴリズムを与えるため、高次元幾何の独創的な活用を主として取り扱う。典型的な応用分野としては、ナッシュ均衡の計算、ページランク最適化、教師付き機械学習とマイニング最適化などがある。理論的成果に加えて、産学官で広く利用でき、実用的な問題サイズが解けるような革新的な並列化ソフトウェアを実装する。

研究成果の概要(英文)：The purpose of this grant was to provide funds to pursue the research goals of the Geometric Computation Laboratory (GCL) at Kyoto University, which I founded in 2010. We are concerned primarily with the ingenious use of high dimensional geometry as the driving force to provide innovative new algorithms for solving previously intractable problems of high impact in engineering and science. Typical application areas include computing Nash equilibria, PageRank optimization, supervised machine learning and mining optimization. In addition to creative new theoretical results, the laboratory will implement innovative highly parallel software to allow the results to be used in academia, industry and the society at large on problems of practical size.

研究分野：情報学

キーワード：計算機科学 離散幾何学 最適化

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.

2 . 研究の目的

In order to concretize these goals I created the Geometric Computation Lab (GCL) at Kyoto University in 2010 using startup funds from JSPS to purchase the initial equipment. I believe that the GCL is the first laboratory of its kind in Japan. Other first class research labs in this area exist in major universities, such as, e.g., ETH (Fukuda and Welzl), TU Berlin (Grotschel and Ziegler), MIT (Demaine and Goemans), McGill (Reed, Shepherd, Vetta) to name a few. My overall goal was to develop a group of equal caliber at Kyoto University. An important feature of our work is that we fully incorporate creative theoretical insights into innovative highly parallelized and easy to use software for wide distribution. Although polyhedral methods have become an important tool in many areas of research in engineering and science, there was relatively little readily available software for the general researcher that exploits massive parallel architecture. My **first goal** was therefore to greatly expand the tools available and computational power available to the general researcher.

An important research topic on polyhedra relates to the complexity of linear programming pivoting methods. Friedmann et al. [2] [5] have brought powerful new tools from game theory and Markov decision processes to bear, and

have given subexponential lower bounds for certain well established rules. My **second goal** was to extend these lower bounds to other history based pivot rules, to determine if matching upper bounds exist and to study the generalization of this approach to more abstract settings that go beyond polyhedral methods, including the computation of Nash equilibria and other linear complementarity problems.

My **third goal** was to find innovative applications of the methods of geometric computation to high impact practical problems. These include supervised machine learning, PageRank optimization and open pit mining optimization. One area of application that we were particularly concerned with is discrete optimization because of the tremendous practical application of results in this area for society.

3 . 研究の方法

The research consisted of 6 subprojects in major research areas that spanned the 4 year grant period: history based pivot rules, ground metric learning, directed cuts and open pit mining, and PageRank optimization, parallelization of the *lrs* vertex enumeration code and extension complexity. In each subproject our objectives were met or exceeded. The successful completion of this ambitious plan depended on a highly talented team of collaborators, including 5 Japanese and 7 foreign researchers, and 2 Japanese graduate students who completed Master's theses in areas related to the project.

4 . 研究成果

The Geometric Computation Lab received a series of high profile visits from established foreign researchers such as: Hans Tiwary (Charles), Oliver Friedmann (Munich), K. Fukuda (ETH), S. Langerman (Bruxelles), David Bremner (UNB), D. Rappaport (Queens), and L. Devroye (McGill). Collaborations with these researchers lead to results in the 6 subprojects that we now summarize.

(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 the paper [9] on a systematic study of these pivot rules on abstract hypercubes. Friedmann and I obtained the first exponential lower bound for USOs and LPs that use Cunningham's history based rule, resulting in the paper [11] that will appear in Math. Programming this year.

(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. Marco Cuturi (Kyoto) and I considered algorithms that can learn the ground metric using only a training set of labelled histograms. We wrote the paper [7] on this that appeared in the Journal of Machine Learning.

(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 [2] that appeared in the Journal of Combinatorial Optimization.

(4) PageRank optimization

Hopcroft-Sheldon introduced PageRank games on directed web graphs, where nodes manipulate links in order to optimize their rank. They defined Nash equilibria (NE) to be graphs where no such unilateral manipulation can improve any individual's rank. Daichi Paku, Kazuo Iwama and I characterized which undirected graphs are NE and gave a fixed parameter tractable algorithm for testing this in polynomial time. We presented this at ISAAC'12 and the subsequent journal paper [6] appeared in Discrete Applied Mathematics.

(5) Multicore version of the *lrs* vertex enumeration code.

In 2012 Roumanis and I released the program *plrs* that is a shared memory

parallelization of *lrs* and tested it with hardware using up to 64 processors [2]. This hardware was obtained using my *kakenhi* funds and was installed at GCL in Kyoto University. Over the grant period this cluster grew to a total of 312 cores. The code *plrs* gave very satisfactory speedups up to about 16 cores but speedups were limited as additional cores were added. Furthermore it was not able to run on the multi-machine cluster at GCL. From 2013 Charles Jordan (Hokkaido) and I started a new parallel implementation, *mplrs*, of *lrs* based on Message Passing Interface (MPI) that runs on clusters of machines. We experimented with various techniques to improve on the load balancing problem encountered with *plrs* for medium to large scale systems. Finally we discovered a very simple technique we call budgeting that gave very good speedups over the entire cluster. This work is reported in [12]-[13].

(6) Extension Complexity

One of the exciting outcomes of the grant was a collaboration project I started with Hans Tiwary on the rapidly emerging field of extension complexity. This subject is concerned with showing the limitations of linear programming in solving NP-hard problems. The collaboration was made possible by JSPS funds which supported three trips to Kyoto University by Tiwary and has resulted in one conference paper and three papers accepted for publication in leading journals in the field.

In our first collaboration we extended earlier results of Fiorini et al. on the extension complexity of the cut polytope and related polyhedra. We first described a lifting argument to show exponential extension complexity for a number of NP-complete problems including subset-sum and three dimensional matching. We then obtained a relationship between the extension complexity of the cut polytope of a graph and that of its graph minors. Using this we were able to show exponential extension complexity for the cut polytope of a large number of graphs, including those used in quantum information and suspensions of cubic planar graphs. This work was initially presented at the prestigious ICALP conference [1]. We extended these results resulting in a journal version [5] that appeared in Mathematical Programming.

In our second paper [3] we proposed a

generalization of the extension complexity of a polyhedron Q . On the one hand it is general enough so that all problems in P can be formulated as linear programs with polynomial size extension complexity. On the other hand it still allows non-polynomial lower bounds to be proved for NP-hard problems independently of whether or not $P=NP$. The generalization, called H-free extension complexity, allows for a set of valid inequalities H to be excluded in computing the extension complexity of Q . We gave results on the H-free extension complexity of hard matching problems (when H are the odd set inequalities) and the traveling salesman problem (when H are the subtour elimination constraints).

In our third and most recent paper [1] we applied the framework we described in [3] to the traveling salesman problem (TSP). It was previously known that the extension complexity of the TSP polytope for the complete graph K_n is exponential in n even if the subtour inequalities are excluded. In this paper we studied the polytopes formed by removing other subsets H of facet defining inequalities of the TSP polytope. In particular, we considered the case when H is either the set of blossom inequalities or the simple comb inequalities. These inequalities are routinely used in cutting plane algorithms for the TSP. We showed that the extension complexity remains exponential even if we exclude these inequalities. In addition we showed that the extension complexity of the polytope formed by all comb inequalities is exponential. In our proofs we introduced a subclass of comb inequalities, called (s,t)-uniform inequalities, which seem to be of independent interest.

Finally Tiwary and I collaborated with David Bremner and Osamu Watanabe to build a compiler that can convert any algorithm written in a basic pseudocode into a linear program. The initial goal here was to find a polynomial size polytope for the matching problem. Rothvoss had previously proved that no such polytope can be an extension of the Edmond's polytope, so our work leads to completely different families of polytopes. The associated paper [10] has been submitted for journal publication. On the practical side, Bremner and I have implemented a prototype of the compiler.

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国内外の別：

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6 . 研究組織

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