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研究課題名（和文）Data Mining for Graphs and Networks via Local Intrinsic Dimensional Modeling

研究課題名（英文）Data Mining for Graphs and Networks via Local Intrinsic Dimensional Modeling

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研究成果の概要（和文）：このコンピュータサイエンスプロジェクトの全体的な目的は、特徴アンサンブル、グラフ、ネットワークなどの複雑なデータタイプの類似性アプリケーションにおける次元の呪いの問題に取り組むことであった。 主な目標：（1）組み合わせデータ型を説明するために内在次元の既存の理論を進歩させること。（2）実証的研究によって理論的意味を確認する。（3）ローカル内在次元理論（LID）の新しい進歩を活用して、データベース、データマイニング、マルチメディア、特にグラフ、ディープニューラルネットワーク、フィーチャアンサンブル、その他の複雑なデータタイプのアプリケーション向けのために効率的で効果的なソリューションを開発する。

研究成果の学術的意義や社会的意義
この研究プロジェクトは、機械学習とデータマイニング分野のトップ国際会議(ICML、ICMR、KDD、SDM)において、５つの影響力のある出版物を生み出した。この研究は、実際に非常に大きな影響を及ぼし、3年未満で、2つの論文が、合計約500件近く引用されるまでに達した。

研究成果の概要（英文）：The overall aim of this computer science project was to tackle the problem of the curse of dimensionality in similarity applications for complex data types such as feature ensembles, graphs and networks, through the further development of practical techniques that recognize and take advantage of local variations in the intrinsic dimensionality of the data. The main goals were: (1) to advance the existing theory of intrinsic dimensionality to account for combinatorial data types; (2) to confirm the theoretical implications by means of empirical study; (3) to exploit new advances in the theory of local intrinsic dimensionality (LID) to develop more efficient and effective solutions for applications of databases, data mining and multimedia, particularly for graphs, deep neural networks, feature ensembles, and other complex data types.

研究分野：data mining, machine learning, similarity search

キーワード：高次元空間　極値理論　データマイニング　機械学種　ニューラルネットワーク

１．研究開始当初の背景

In the era of Big Data, data volumes have become so enormous and so complex as to preclude processing using traditional applications. For similarity search and retrieval, as well as many other fundamental operations in such areas as data mining, machine learning, multimedia, recommendation systems, and bioinformatics, the efficiency and effectiveness of software implementations depends crucially on the interplay between measures of data similarity and the features (or attributes) by which data objects are represented. For such applications (which we refer here to as *similarity applications*), features are often sought so as to provide the best possible coverage across a range of anticipated queries. However, for any given query, only a relatively small number of features may turn out to be relevant. When the number of features (the data *dimensionality*) is high, the errors introduced into similarity measurements by the many irrelevant feature attributes can completely overwhelm the contributions of the relevant features. As the dimensionality of data increases, the discriminative ability of similarity measures diminishes to the point where techniques that depend on search lose their effectiveness. This phenomenon, of profound importance to computing, is commonly referred to as the *curse of dimensionality*.

Although high-dimensional data sets are generally difficult to process, it is not always the case. Data sets of high dimensionality can often be searched and analyzed relatively easily, provided that the so-called *intrinsic dimensionality* is low. The intrinsic dimensionality of a dataset can loosely be regarded as the number of latent variables needed to describe a data set: this could be the number of 'relevant' or 'non-redundant' features, or the degrees of freedom of a distribution that accurately models the data. Over the past decades, very many formal characterizations of the intrinsic dimensionality of data sets have been proposed within the statistical and machine learning research communities.

Until the beginning of the project, the theory and practice of intrinsic dimensionality had been limited to global approaches, where the intrinsic dimensionality is expressed as a single value for an entire dataset. However, this does not fit well with the user's experience of the data, where interest may be focused on a specific query result or a specific data cluster. Just as data is often modeled as a mixture of underlying distributions, data sets have regions of varying intrinsic dimensionality – and these local variations should be modeled theoretically and exploited in practice.

In 2013 the *local intrinsic dimension* (LID) was introduced so as to model the behavior of distance distributions within the vicinity of points of interest (such as query objects in indexing, or test objects in machine learning). The LID model is comprehensive and general, and practical estimators for LID existed. Since its first appearance, LID had already made an impact in practice, in guiding the design and performance analysis of a wide variety of state-of-the-art solutions for similarity applications.

The LID model is a model of complexity that assesses growth rate in continuous processes, such as of expected neighborhood sizes in similarity applications, or of probability measure in statistical modeling. Despite its successes with continuous data models, LID in its current form cannot be directly applied to discrete data such as graphs, networks, or lists. There are many important application areas where the natural data representations are discrete, and for which there are no satisfactory measures of local query result complexity. For social networks and deep neural network classifiers represented as graphs, or recommender systems and search systems that aggregate ranked lists of data objects or collections of feature sets, direct measures of the complexity of similarity query results are difficult to compute and to apply, due to their reliance on the discrete combinatorial structure of the underlying data representations. For this reason, researchers have been interested in developing continuous generation models for certain classes of structured data, where instances can be thought of as having been constructed according to a particular random generation scheme. Examples of random generation include: a form of densely-connected graph for cluster structure; models of scale-free graphs for social networks; and infinite-neuron layer representations for the theoretical analysis of certain aspects of deep neural network classification.

The main scientific questions to be addressed by this project were as follows. For applications in machine learning, data mining, and other areas in which similarity information is used, how can important structured data types be modeled continuously so as to best support generalization from instances (such as in unsupervised learning from data sets, or supervised learning from training sets)? And can the theory of local intrinsic dimensionality be extended so as to exploit these models in practice?

２．研究の目的

The overall goal of this project was to tackle the curse of dimensionality in similarity applications for structured data types such as feature ensembles, ranked lists, graphs and networks, through the further development of practical techniques take advantage of local variations in the intrinsic dimensionality of the data. This was to be done through the extension of the LID theory so as to account for continuous models of structured data and the interactions among combination of features, followed by exploitation of the extended LID model to improve the performance of similarity applications on such data beyond that of current state-of-the-art methods. Within this context, the goals of the project can be summarized as follows:

1. To advance the existing theory of intrinsic dimensionality to account for complex data types, in which continuous generative models are developed and analyzed for such types as feature ensembles, graphs and classification networks;
2. To confirm the theoretical implications by means of empirical study of the relationship between local ID and the performance issues that surround similarity applications;
3. To exploit new advances in the theory of LID to develop more efficient and effective solutions for applications of databases, data mining and multimedia, particularly for graphs, deep neural networks, feature ensembles, and other complex data types;
4. To make these technical innovations available to researchers and practitioners through their integration into practical systems for search and analysis of data, as well as through publication in top-level international journals and conference proceedings.
5. To further promote the interdisciplinary international research community focused on the issues of dimensionality and scalability in the context of databases, machine learning, data mining, and multimedia.

３．研究の方法

The project was a 3-year international collaboration among 6 main participants (the Principal Investigator plus 5 international Research Collaborators), each one a member of a different research institute or university. Collectively, the participants have expertise that spans the areas of computer science that are touched by the curse of dimensionality, including: theory, algorithms, and similarity applications for databases, machine learning and AI (including deep learning), data mining, and multimedia (search and indexing, clustering, outlier detection, feature selection). Within the first year, we planned to expand the theory of LID to account for the interactions among combinations of features, and to show that decompositions of weighted LID can be used to determine low-dimensional local data projections using an approach resembling that of PCA. In the area of graphs and networks in learning contexts, the goal for the first year was to investigate the phenomenon of adversarial attack and deep neural network classification. In later years of the project, we planned to extend the work to follow-on projects in intrinsic dimensionality for complex data applications, with a particular emphasis on deep learning and graph analysis. In all three years of the project, new techniques were to first be applied to simple continuous data types where appropriate, so as to assess the feasibility of extending them to complex data types.

The following lists the expertise that each member brought to the project when it began in 2018 (current affiliations and positions are shown).

- Vis. Prof. Michael E. Houle, National Institute of Informatics (NII), Japan, PI: theoretical computer science, algorithms, data mining, indexing, similarity applications, computational geometry. His main expertise was in the design and analysis of algorithms for similarity search, clustering, outlier detection and feature selection that exploit intrinsic dimensionality.
- Dr. Laurent Amsaleg, CNRS-IRISA Rennes, France, RC: multimedia databases, multidimensional indexing, content-based retrieval, database security and privacy. Dr. Amsaleg had developed practical multimedia indexing systems handling billions of images, represented by millions of features. He had collaborated with Houle on the development of estimators of LID as well as other similarity applications.
- Assoc. Prof. Miloš Radovanović, University of Novi Sad, Serbia, RC: data mining, clustering, experimental validation. Prof. Radovanović is the foremost authority on the hubness phenomenon (implicitly addressed by the LID model), as well as algorithms for data clustering which exploit it.
- Prof. James Bailey, University of Melbourne, Australia, RC: data mining, machine learning, clustering, outlier detection. Prof. Bailey had recently collaborated with Houle, Amsaleg, and Radovanović on an analysis of adversarial attack, and with Houle on measuring functional dependency, both using LID.
- Prof. Arthur Zimek, University of Southern Denmark (USD), Denmark, RC: data mining, clustering, outlier detection. Prof. Zimek is a leading authority in these areas, having co-authored several prominent surveys. Prof. Zimek had had several joint publications with the PI in the area of data mining. While at the University of Munich (LMU) in Germany, Prof. Zimek co-created the well-known ELKI data mining application development platform.
- Prof. Vincent Oria, New Jersey Institute of Technology (NJIT), USA, RC: databases, multimedia indexing. Prof. Oria had collaborated closely with the PI on applications of ID to adaptive similarity queries and subspace similarity search.

Each of these main team members was responsible for organizing contributions to the project drawn from their own research collaborators and students.

４．研究成果

Of the goals laid out at the beginning of the project, we have fully met our objectives with respect to the 3 main research goals. The 4th and 5th goals were only partially met, due to the severe difficulties in implementation and publication during the last year of the project (due to illness, to the lack of availability of students supervised by project members, and on international travel restrictions). In particular, we were not able to fully meet our objectives of integrating our research results into practical systems (due to the lack of availability of students), and in hosting a third international meeting on the topic of LID and its applications (due to the restrictions on travel).

The main discovery of the project is that the local ID model can be used to guide and explain, in a very useful and intuitive way, some of the important characteristics of learning and classification using deep neural networks. The most important outcomes with the greatest impact to date are:

- Publication of a refereed paper at the top-tier International Conference on Learning Representations (ICLR 2018). This paper presented a characterization of corrupted examples in adversarial attack on classification systems, and a practical detection method, based on the LID model central to this project. (Acceptance rate: 2.5%. Number of citations to date, in 3 years: 317.)
- Publication of a refereed paper at the top-tier International Conference on Machine Learning (ICML 2018). This paper demonstrated that the progress of learning in deep neural network (DNN) classifiers is strongly correlated with a drop in LID at the deep feature level, and showed how to use this effect to prevent overtraining and overfitting to data. (World first in automatic detection and avoidance of overtraining during DNN learning. Number of citations to date, in 3 years: 172.)
- Publication of a refereed paper at the top-tier ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (KDD 2019). This paper presented a technique for generating more realistic synthetic neighbors for the purpose of explainability of learned solutions in deep learning. The improvements to explainability were due to the use of the local intrinsic dimensionality (LID) model central to this project. (Acceptance rate: 14%.)
- Publication of a refereed paper at the top-tier SIAM International Conference on Data Mining (SDM 2019). This paper proposed an estimator for LID that makes use of all pairwise distances within a local neighborhood sample. This use of full similarity neighborhoods allows significantly higher quality of estimation within more tightly-focused neighborhoods. This estimator targets applications in anomaly and outlier detection in data mining, among others. (Acceptance rate: 23%.)
- A refereed publication at a top international conference (SDM 2021) on the use of local intrinsic dimensionality (LID) on the problem of out of-distribution detection in deep learning. LID is used as a feature to characterize the data subspaces formed by data samples and their corresponding reconstruction by autoencoders.
- A refereed publication in early 2021 in the top journal IEEE Transactions on Information Forensics and Security, in which the full details of a theoretical analysis is given showing that the vulnerability of classification to adversarial perturbation increases as the local intrinsic dimensionality rises.

Other highlights within the project outcomes include:

- 2018: Refereed publications at international conferences: (3 at SISAP 2018) correlation between LID and outlierness, the use of LID in accelerating the performance of data fingerprinting, and an adaptation of LID to model the local growth rate of search neighborhoods within graphs; (1 at WIMS 2018) examination of the effect of reverse neighborhood imbalance in similarity graph construction.
- 2019: 2 refereed publications at international venues: (SISAP 2019 conference) the use of decompositions of LID to determine relevant local data subspaces; (IJAIT journal) an empirical analysis of the NN-descent similarity search method, in terms of local neighborhood imbalance (the hubness phenomenon, related to extreme LID scores). 2 unrefereed publications (arXiv): a full version of the SISAP 2019 paper; and work in progress on the use of an LID-based regularization for improving the quality of GAN-based deep learning.
- A refereed international conference publication (at SISAP 2020) on a theoretical aspect of the LID model, on the use of similarity measures in determining density ratios between two localities in distance distributions. This work lays the first theoretical and practical foundations for density-based outlier detection that properly takes into account the effects of variation in local intrinsic dimension. Preliminary implementations show very competitive performance against the state of the art; however, the work has not yet been published.

The funding for this project was intended to support collaborative research visits among partners from Japan and 5 countries (Australia, Denmark, France, Serbia, and the United States), and conference travel for the reporting of research results. However, as travel has been disrupted due to the COVID-19 pandemic, the research funds for 2020 have gone unused, and (due to difficult circumstances for most of the participants) projects have been delayed. For this reason, most of the projects planned for 2020 will fully resume only after the end of the pandemic. Nevertheless, we are pleased that the project was able to meet its main objectives regardless.

5．主な発表論文等

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1．著者名 Xingjun Ma, Bo Li, Yisen Wang, Sarah M. Erfani, Sudanthi N. R. Wijewickrema, Grant Schoenebeck, Dawn Song, Michael E. Houle, James Bailey	4．巻 6
2．論文標題 Characterizing Adversarial Subspaces Using Local Intrinsic Dimensionality	5．発行年 2018年
3．雑誌名 6th International Conference on Learning Representations (ICLR 2018), CoRR abs/1801.02613	6．最初と最後の頁 1～15
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〔学会発表〕　計0件

〔図書〕　計0件

〔産業財産権〕

〔その他〕

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6．研究組織

	氏名 （ローマ字氏名） （研究者番号）	所属研究機関・部局・職 （機関番号）	備考

7．科研費を使用して開催した国際研究集会

〔国際研究集会〕　計0件

8．本研究に関連して実施した国際共同研究の実施状況

共同研究相手国	相手方研究機関			
オーストラリア	University of Melbourne			
フランス	CNRS / IRISA Rennes	INRIA / IRISA Rennes		
米国	New Jersey Institute of Technology			
デンマーク	University of Southern Denmark			
セルビア	University of Novi Sad			