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FEATURE STORY

Mastering Data Science - semantic understanding of multifarious big data and its social implementation

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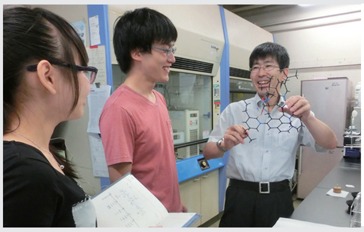
Research Highlights



Pick Up

Mastering Data Science - semantic understanding of multifarious big data and its social implementation

Masaki Aono

Nowadays it is common for large amounts of data to being stored and used on the internet via SNS and other online data repositories. Data science technology, including information retrieval and data mining (which allows you to search and extract latent but potentially important pieces of information from the data), is vital in an era flooded by so-called "big data". Professor Masaki Aono has been a leading figure in knowledge data engineering research since the 1980's, and it is his goal to keep conducting challenging research in the area of data science. Professor Aono started with 3D shape retrieval, gradually incorporating various popular state-of-the-art technologies ranging from multivariate data analysis and traditional machine learning to deep learning.

Interview and report by Madoka Tainaka

World Champions in a Plant Identifying Contest

In 2016, a research team led by Professor Masaki Aono won first place for identification accuracy in an international contest called "PlantCLEF2016". PlantCLEF2016 is a competition where participants use image processing technology to automatically classify 1,000 plants from photographic images.

Professor Aono tells us "actually our research team has been participating in the international image annotation competition, ImageCLEF since 2012. The focus of this year's PlantCLEF contest was on plants. You had to guess each plant's name based on some crowd-sourced photos, but it's quite a difficult task. For example, some photos include a human hand or a tripod, meaning that the data given to participants naturally includes "noise" completely unrelated to plants. Furthermore, the photos could be closeups, very tiny or even out of focus. I guess the reason we could come home with the first prize is that we were able to come up with a way of extracting the 'features' from metadata which helped us to gain more correct answers in spite of the formidable task."

As the amount of data used in the contests is increasing, the research lab has been developing their hand-engineered GPU (Graphics Processing Unit) machines every year, and this time they incorporated deep learning to exploit the full capacity of the GPU machines. In fact, deep learning is a technology that has been gaining attention in the field of AI.

However, the victory by Professor Aono's team does not only come down to deep learning.

"In 2014, we also won the first prize at the ImageCLEF I mentioned earlier, but that time we used ontology and traditional machine learning rather than deep learning. Ontology is a hierarchical system that explicitly expresses a concept and systematically describes the relationship between the concepts. In other words, it is a vocabulary set that the computer uses to successfully orchestrate texts and images. By taking advantage of ontology, we managed to achieve a high level of accurate annotation to images, while other teams using deep learning could not." the professor explains.

Fig.1 Guess each plant's name from given a bunch of the crowdsourced photos.
CREDIT: Copyright © PlantCLEF 2016

The Key is How to Combine Features

Professor Aono says that their team's strength lies in their 'feature combination technology'. A feature is a numerical expression of the characteristics or attributes observed in the target data. Even in ontology, it is crucial to configure the feature correctly. Up until now, the feature was extracted manually, which is called "hand-crafted features", but with the increase of the amount of data the team began to adopt deep learning to complement the proposed features.

"We came up with a new method for deep learning as well. Out of the 100,000 photos in the training data, we gave the computer various types of images – images that were out of focus, images that were zoomed in on different parts – so that it would be able to deal with any kind of images. We also incorporated the date and time stamps that were added to the data, which were allowed to be used as metadata. From this we could infer that images taken at almost the same time were most likely to be of the same plant. In the contest in 2016, somehow no other teams tried to use this metadata. In fact, ironically for the other teams, it was the use of this metadata that improved our performance and made it possible for us to become world champions."

"Regarding an underlying technology which aids in the extraction of features in deep learning called convolution, the team came up with some new ideas to change the internal structure, which gave them another advantage over the other teams. The credit for this goes to a clever exchange (2nd year masters) student from Malaysia. The results were even featured in Springer's international journal 'Multimedia Tools and Applications'."

Setting yourself apart is an important task in the competitive world of data engineering processing research. You especially cannot hope to compete with big companies such as Google, Facebook and other IT companies that have access to enormous amounts of data and resources for their research development. This is the reason Professor Aono first chose to work with the 3D shapes retrieval which, as a less popular research domain has not been substantially focused on by big companies but is yet manageable in terms of difficulty.

"Three-dimensional CAD (Computer-Aided Design) is being used in a variety of situations, from the design of machine parts to architectural design, to CG creation, but currently time and skill are two crucial elements in creating the underlying model for the geometric shapes. We developed technology that uses an existing database of 3D shapes to find models that are similar to 2D images or 3D shapes acquired by using commercially available motion sensors such as Kinect or sketches with high precision. If you can search for similar models, there is no need to configure the model from scratch which improves the efficiency and means that even novices can design complicated parts using CAD."

This system's retrieval is currently the world's most accurate (amongst the methods of searching similar 3D shapes with no prior supervised learning) and Professor Aono tells us he is in the middle of applying for several new patents, for some of which the technology is being transferred to companies that collaborated in the research.

I want to put my research results to good use in the real world, such as self-driving cars and agriculture.

In addition, Professor Aono is also working on research that gathers chronological data that can be collected from different types of sensors, and predicts what may happen by learning in advance.

"For example, I am conducting research into controlling the environment of a greenhouse to maximize the amount of vegetables and fruits that can be harvested by equipping the greenhouse with sensors that measure humidity, moisture, sunlight, CO_2 etc., then wirelessly collecting and analyzing the data. In the past, I conducted demonstration experiments on greenhouses used to suggest the best control over greenhouse environment in order to maximize the yield of tomatoes."

In regard to the processing of chronological data, the professor is also pursuing research into BCI (Brain Computer Interface), using data from the human brain to predict a person's psychological state or to allow for communication with a computer simply by thinking. He is also beginning research that uses LSTM (Long Short-Term Memory), a type of deep learning, where both long and short-term chronological data can be handled. This technique can be used, for example, to guess an author of a book from a piece of writing, or automatically create a piece of writing in the style of a specific author.

On the other hand, his research on scene graphs for automatically adding notes to an image is also interesting. A scene graph is a method of displaying the relationship either between two objects or between an object and the attribute, with a so-called 'directed graph structure' (a graph composed of nodes and directed edges).

"For example, if we can automatically extract objects in an image such as roads, trees, cars, the sky etc. and add notes about the relationship, it would become possible for the computer to answer questions such as what kind of trees there are, whether it's sunny, if there are any obstructions in front of us, etc.

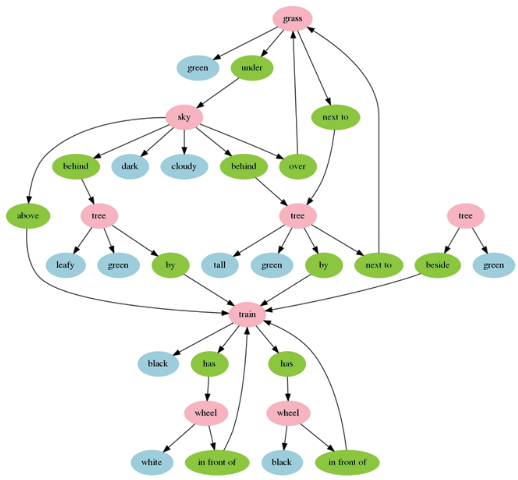


Fig.3 Example of a scene graph:. a red-green-red path indicates the relationship between two nodes, where the type of the relation is represented by the text in green node. A red-blue path indicates the relationship between an object and the attribute.

If we continue to progress with this research, we could use it in car navigation systems to give commands such as 'turn right at the brick building in front of you'. If we could add notes to the constantly changing scenery, I think it may help develop self-driving cars in the future," says Professor Aono.

"I'm troubled by the amount of things I want to do," adds the professor. His research includes a number of different topics, all of which are building blocks critical to the development of increasingly influential field of AI. No doubt the Professor will continue to contribute actively to this effort in the future.

[Reporter's Note]

Professor Aono started working at IBM after graduating from Tokyo University with a Master's degree in CG and CAD. From the late 1990's he started looking at information retrieval. He became a professor at Toyohashi University of Technology in 2003, and accelerated his research. "I want to construct a system that can correctly identify things even better than a human specialist." That is the motivation behind his research.

The Professor feels that he gets his love of nature, including an obsession with classification, from his father, who was the former curator of the Kurashiki Museum of National History in Okayama Prefecture. On his days off he enjoys taking photos of flowers and birds. Recently he succeeded in taking a photo of a red-flanked bluetail, a photo he had been chasing after for a long time. "One day I would like to try and use data processing to identify birds and insects." The professor has an endless curiosity. Professor Aono's 'search for a bluebird' continues inside his research.

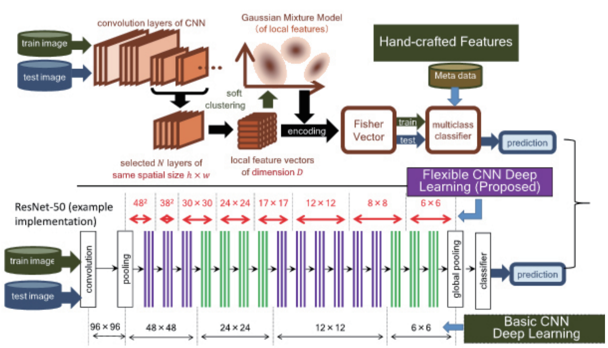


Fig.2 Proposed deep learning approach of Convolutional Neural Network (CNN) and Residual Network (ResNet)

3Dや画像、映像、テキストなど、多種多様なデータ処理を究める

近年、SNSやオンラインのデータレポジトリなどWeb上に、多種多様かつ大量のデジタルデータが蓄積され、利用されている。そのデータ活用に欠かせないのが、情報検索やデータから有用な情報を取り出すデータマイニングなどの処理技術だ。青野雅樹教授は、1980年代からこうした知的なデータ処理分野の研究を手がけてきた第一人者である。三次元の形状類似検索をはじめ、画像、映像、テキストと、多種多様なデータを対象に、深層学習などの先端技術も取り入れながらデータ処理の精度向上を目指している。

植物鑑定のコンテストで世界一に

2016年、青野雅樹教授が率いる研究チームが、"PlantCLEF2016"と呼ばれる国際コンテストで世界第1位の鑑定精度を獲得した。PlantCLEF2016では、1000種類の植物の写真画像から、画像処理技術などを使って種類を自動で鑑定するコンテストだ。
「実は、我々のチームは2012年からImageCLEFという画像検索の国際コンテストに参加していて、今回のPlantCLEFはその中でも植物に特化したコンテストです。クラウドソーシングで集められた写真から植物の名前を当てるのですが、けっこう難しい課題なんですよ。たとえば、植物とともに人間の手や脚が写っている写真や、樹肌のアップ、あるいは遠景写真なども混ざっています。コンテストで我々がトップになったのは、"特徴量"の抽出の仕方に工夫を凝らすことで、過酷なタスクに対しても正答率を上げることができたからだと思います」と青野教授は説明する。
年々、こうしたコンテストで扱うデータ量は増大しているため、研究室では手作りのGPU（Graphics Processing Unit）マシンを年々増やし、今回はさらに、近年、AIの分野で注目されている深層学習も取り入れた。ただし、青野教授チームの勝利は、深層学習だけによるものではない。
「2014年に、先のImageCLEFでも我々は世界1位を獲得しているのですが、このときは深層学習ではなく、オントロジーを使った、通常の機械学習を採用しました。オントロジーというのは、概念を明示的に表現し、それらの関係を体系的に記述した階層的な概念体系のこと。つまり、コンピュータがテキストや画像をうまく処理できるようにするための語彙のセットのことです。これをうまく使うことで、深層学習を使った他チームよりも高精度を達成しました」と青野教授は言う。

肝となるのは特徴量をいかに組み合わせるか

青野教授は、自らのチームの強みを「特徴量の組み合の技」にあると言う。特徴量とは、学習データにどのような特徴があるのかを数値化したもののこと。オントロジーを使う場合でも、そこから特徴量をうまく設計することが肝要になる。従来、この特徴量の抽出は手作業で行っていたが、データ量の増大に伴い、特徴量を自動で抽出するために、ここへきて深層学習を採用し始めた。

「深層学習にも工夫を凝らしました。10万枚ほどの学習用の訓練データの中にはピンボケ写真や部分のアップなどさまざまなものを入れて、どんな画像にも対応できるようにしました。また、メタデータとして利用が許されていた、データに付与された日時も取り入れました。ほぼ同時刻に撮られた画像は同じ植物だろうと推定するわけです。2016年当時のコンテストでは他のチームは、このメタデータを利用しようとしませんでした。実は、他のチームにとっては皮肉なことに、このメタデータの利用が性能をかなり押し上げ、我々のチームが世界一になったようです。

さらに、深層学習において特徴量の抽出に役立つ畳み込みという手法についても、その中身の構造を変える新しいアイデアを生み出して、他チームとの差別化を図りました。このアイデアには、当時、修士2年だった優秀なマレーシア人の留学生が大活躍しました。この成果は、Springer社の"Multimedia Tools and Applications"という国際ジャーナルにも採択されました」

競争の激しいデータ処理研究の分野で、差別化は重要な課題だ。とくに膨大なデータと資産を背景に研究開発を進めているGoogleやFacebookなどのIT企業と真っ向から勝負を挑んでも太刀打ちできない。そうしたことから、青野教授が最初に手がけたのは、難しいがゆえにあまり研究されていない三次元の形状類似検索だった。

「現在、機械部品の設計をはじめ、建築設計やCGの制作などの現場など、さまざまな場面で三次元CAD（Computer-Aided Design）が使われていますが、そうした幾何学形状のモデルをゼロから制作するには、手間と熟練の技が欠かせません。そこで、既存の三次元形状モデルを蓄積したデータベースから、Kinectなど市販のモーションセンサデバイスを使って得た3D画像や形状モデル、スケッチから似たモデルを高精度で検索する技術を開発しました。似た形状モデルが検索できれば、ゼロから設計する必要がなくなり、効率化が図れるうえに、新人でもCADで複雑な部品の設計ができるようになります」

このシステムの検索精度は現時点で（事前学習を要しない3D形状類似検索手法で）世界一を誇り、新たないくつかの特許を出願中で、その一部は共同研究先の企業に技術移転中だという。

研究成果を自動運転や農業など、実社会に役立てたい

その他にも青野教授は、各種センサから得られる時系列データを収集して、事前に学習することで、これから起こり得る事象を予測する研究にも注力している。「たとえば、温室内に温度や水分、日射量、CO_2などを測るセンサを配備し、無線でデータを集めて解析し、温室内の野菜や果物の収穫量が最大になるように温室の環境を制御する研究も行っています。これまで、トマトの温室栽培で実証実験をしたことがあります」

時系列データの処理に関しては、ヒトの脳のデータを計測して、どのような心理状態にあるのかの予測や、考えただけでコンピュータとコミュニケーションができるBCI（Brain Computer Interface）の研究も手がける。さらに、深層学習の一つであるLSTM（long-short Term Memory）を使って、長期の時系列データの学習に役立てることで、例えば文章から作家を推定したり、特定の作家風の文章を自動で生成したりといった研究も始めている。

一方、与えられた画像に自動で注釈をつけるシーングラフに関する研究も面白い。シーングラフとは、対象物間の関係を、木構造と呼ばれるグラフ（点と辺で構成される図形）で示す手法である。「たとえば、画像に写っている道や木、車、空といった対象物を自動で抽出して、その関係性に注釈をつけることができれば、これは何の木なのか、今日は晴れているのかどうか、目の前に障害物がないかどうかといったQ＆Aに答えることが可能になります。

さらにこの研究を進めることができれば、『正面のレンガの建物があるT字路で右折してください』といったように、カーナビに使うこともできるでしょう。時事刻々と変化する風景に応じて注釈をつけることができれば、将来的には自動運転にも役立てられるのではないかと考えています」と青野教授。

「やりたいことが多くて困ってしまいますね」と青野教授が言うように研究は多岐にわたるが、いずれも、現在、社会を大きく変えるとして注目されるAIの進展に欠かせない基盤技術である。今後のさらなる成果に期待したい。

（取材･文＝田井中麻都佳）

取材後記

青野教授は、大学卒業後、IBMに就職し、CGやCADの研究を経て、1990年代後半から情報検索の研究を手がけている。2003年から豊橋技科大の教授となり、研究を加速させてきた。「専門家でも見分けるのが難しいようなものを、正確に言い当てるシステムを構築したい」というのが研究のモチベーションだ。

実は、お父様は岡山県倉敷市の自然史博物館の元館長さんで、鑑定へのこだわりや自然への愛着は父親譲りだという。休日は、草花や鳥の写真撮影を楽しむ。先日、長年追い求めていた青い鳥「ルリビタキ」の撮影に成功した。「いずれ、データ処理で鳥や虫の鑑定もやってみたいですね」と、探究心は尽きない。青野教授の研究における「青い鳥」探しはまだまだ続く。

Researcher Profile

Dr. Masaki Aono

Dr. Masaki Aono received the BS and MS degrees from the Department of Information Science from the University of Tokyo, the PhD degree from the Department of Computer Science at Rensselaer Polytechnic Institute, New York. He was with the IBM Tokyo Research Laboratory from 1984 to 2003. In 2002 and 2003, he was a visiting teacher at Waseda University. He is currently a professor at the Graduate School of Computer Science and Engineering Department, Toyohashi University of Technology.

Reporter Profile

Madoka Tainaka is a freelance editor, writer and interpreter. She graduated in Law from Chuo University, Japan. She served as a chief editor of "Nature Interface" magazine, a committee for the promotion of Information and Science Technology at MEXT (Ministry of Education, Culture, Sports, Science and Technology).

Discovery of “Helical Molecular Glue”

A counterclockwise-helical molecule glues two structurally-different clockwise-helical molecules together

By Hideto Tsuji

Professor Hideto Tsuji and his colleagues have made a world-first discovery of the “molecular glue” action of a counterclockwise-helical molecule to glue two structurally-different clockwise-helical molecules together. This discovery was announced on March 24, 2017 in Scientific Reports. To bind two polymers coiled in the same direction was previously considered impossible. Consequently, the degree of freedom in polymer combination has increased, and development of new polymer materials with various properties has become possible.

Professor Hideto Tsuji (2nd from right, front raw) with his laboratory members

The research group led by Professor Hideto Tsuji conducts basic and applied researches on biodegradable polymers derived from renewable resources such as corn or potato starch. The group mainly studies a typical biodegradable polymer poly (lactic acid). Poly (lactic acid) is hydrolyzed and degraded in the human body and the resulting lactic acid is metabolized without causing adverse effects to the body. Because of this advantage, poly (lactic acid) is used in medical applications as a scaffold material for tissue regeneration and also in environmental applications.

Poly (lactic acid) contains an asymmetric carbon and therefore occurs either as the L- or D- enantiomer, namely poly (L-lactic acid) or poly (D-lactic acid) (Fig. 1). Since the interaction between different enantiomers (i.e. between L and D) is stronger than that between the same enantiomers (e.g. between D and D), blending the two enantiomers results in co-crystallization of an L-enantiomer and a D-enantiomer (this phenomenon is also called stereocomplex formation). The stereocomplex has a higher melting point, better mechanical properties, and higher heat resistance and hydrolysis resistance than those of their constituent enantiomers, and therefore the stereocomplex may have wider applications than those of conventional biodegradable materials. Under these circumstances, stereocomplex formation between poly (lactic acid) has been actively researched in recent years.

L-poly (lactic acid) is counterclockwise-helical, and D-poly (lactic acid) is clockwise-helical. Therefore, the fact that L-poly (lactic acid) and D-poly(lactic acid) form a stereocomplex together indicates that a counterclockwise-helical molecule

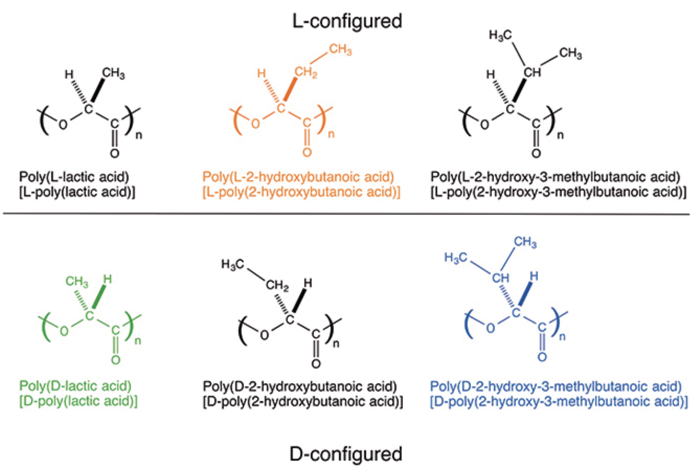


Fig.1 Molecular structures of unsubstituted and substituted poly (lactic acid). Tsuji, H. et al. Configurational Molecular Glue: One Optically Active Polymer Attracts Two Oppositely Configured Optically Active Polymers. Sci. Rep. 7, 45170; doi: 10.1038/srep45170 (2017).

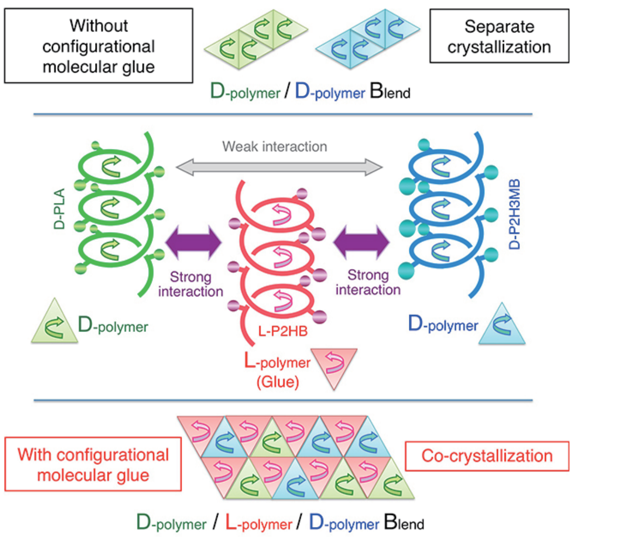


Fig.2 Helical molecular glue. Tsuji, H. et al. Configurational Molecular Glue: One Optically Active Polymer Attracts Two Oppositely Configured Optically Active Polymers. Sci. Rep. 7, 45170; doi: 10.1038/srep45170 (2017).

and a clockwise-helical molecule are strongly attracted to each other. Tsuji et al. have also discovered that blending the L- and D-enantiomers of poly (2-hydroxybutanoic acid) (Fig.1) (a poly (lactic acid) with its methyl group replaced by an ethyl group) results in stereocomplex formation as well. In addition, there are reports of the same phenomena occurring to poly (2-hydroxy-3-methylbutanoic acid) (Fig.1) (a poly (lactic acid) with its methyl group replaced by an isopropyl group) and occurring even between poly (lactic acid) with different side chains (for example, between L-poly (lactic acid) and D-poly (2-hydroxybutanoic acid)). All these phenomena indicate the presence of strong interaction between a counterclockwise-helical molecule and a clockwise-helical molecule.

This time, Tsuji et al. have discovered that a counterclockwise-helical molecule can glue two structurally-different clockwise-helical molecules that would not otherwise bind together (Fig.2). This finding indicates that a clockwise-helical molecule may have a similar effect on two structurally-different counterclockwise-helical molecules. Through experiment using D-poly (lactic acid), L-poly (2-hydroxybutanoic acid), and D-poly (2-hydroxy-3-methylbutanoic acid), Tsuji et al. have made a world first breakthrough by demonstrating that counterclockwise-helical L-poly (2-hydroxybutanoic acid) acts as "helical molecular glue" to glue clockwise-helical D-poly (lactic acid) and clockwise-helical D-poly (2-hydroxy-3-methylbutanoic acid). This process co-crystallizes these two D-molecules which would normally resist co-crystalization. This finding has opened the door to binding various polymers that are coiled in the same direction. Now that the degree of freedom in polymer combination has increased, development of new polymer materials with various properties has become possible.

This work was supported by
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Reference

Hideto Tsuji, Soma Noda, Takayuki Kimura, Tadashi Sobue, and Yuki Arakawa, Configurational Molecular Glue: One Optically Active Polymer Attracts Two Oppositely Configured Optically Active Polymers, Scientific Reports, vol. 7, Article number 45170 (2017).
http://www.nature.com/articles/srep45170

Human Pose Estimation for Care Robots Using Deep Learning

Efficient generation method of big data for pose estimation

By Jun Miura

A research group led by Professor Jun Miura has developed a method to estimate various poses using deep learning with depth data alone. Although it requires a large volume of data, the group has realized a technology which efficiently generates data using computer graphics and motion capture technologies. This data is freely available, and expected to contribute to the progress of research across a wide range of related fields.

Given the backdrop of declining birthrates, an aging population, and a lack of nursing or care staff, there is an increasing expectation that care robots will be required to meet society's needs. It is anticipated, for example, that robots will be used to check the condition of the residents while patrolling nursing homes and other such facilities. When evaluating a person's condition, while an initial estimation of the pose (standing, sitting, fallen, etc.) is useful, most methods to date have utilized images. These methods face challenges such as privacy issues, and difficulties concerning application within darkly lit spaces. As such, the research group (Kaichiro Nishi, a 2016 master's program graduate, and Professor Miura) has developed a method of pose recognition using depth data alone (Fig.1).

For poses such as upright positions and sitting positions, where body parts are able to be recognized relatively easily, methods and instruments which can estimate poses with high precision are available. In the case of care, however, it is necessary to recognize various poses, such as a recumbent position (the state of lying down) and a crouching position, which has posed a challenge up until now. Along with the recent progress of deep learning (a technique using a multistage neural network), the development of a method to estimate complex poses using images is advancing. Although deep learning requires preparation of a large amount of training data, in the case of image data, it is relatively easy for a person to see each part in an image and identify it, with some datasets also having been made open to the public. In the case of depth data, however, it is difficult to see the boundaries of parts, making it difficult to generate training data.

As such, this research has established a method to generate a large amount of training data by combining computer graphics (CG) technology and motion capture technology (Fig. 2). This method first creates CG data of various body shapes. Next, it adds to the data information of each part (11 parts including a head part, a torso part, and a right upper arm part), and skeleton information including each joint position. This makes it possible to make CG models take arbitrary poses simply by giving the joint angles using a motion capture system. Fig.3 shows an example of generating data for various sitting poses.

By using this developed method, training data can be generated corresponding to a combination of persons with arbitrary body shapes, and arbitrary poses. So far, we have created and released a total of about 100,000 pieces of data, both for sitting positions (with/without occlusions), and for several poses in a recumbent positions. This data is freely available for research purposes (http://www.aisl.cs.tut.ac.jp/database_HDIBPL.html). In the future, we will release human models and detailed procedures for data generation so that everyone can make data easily by using them. We hope that this will contribute to the progress of the related fields.

The result of this research was published in Pattern Recognition on June 3, 2017.

This research was partially supported by JSPS Kakenhi (Grants-in-Aid for Scientific Research) No. 25280093.

Reference

Kaichiro Nishi and Jun Miura (2017). Generation of human depth images with body part labels for complex human pose recognition, Pattern Recognition,
http://dx.doi.org/10.1016/j.patcog.2017.06.006

Fig.1 Example of pose estimation using depth data:
Left: Experiment scene (this image is not used for estimation), Center: Depth data corresponding to the extracted person region, Right: Estimation result (the colors correspond to each part of the body

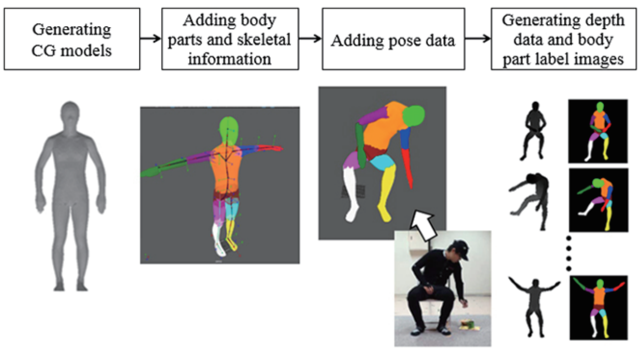


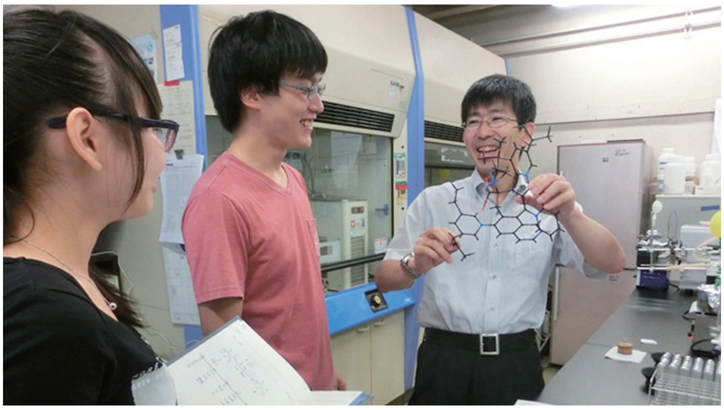
Fig.2 Procedure of generating training data

Fig.3 Example of generating training data for various sitting positions. First row: body part label images, Second row: depth data

The World First Asymmetric Synthesis of Halogenated Compounds from Carboxylic Acids

By Kazutaka Shibatomi

A research team at Toyohashi University of Technology has developed a new reaction to produce chlorinated compounds with high isomeric purity. Such compounds are important building blocks for target molecules. However the molecules come in left- and right-handed versions (enantiomers). They can be produced from carboxylic acids, by replacing acid with chlorine. Although conventional methods produce equal mixtures of both isomers the new method with a chiral amine catalyst specifically yields the desired isomer.



Associate Professor Kazutaka Shibatomi (right) with his students

Toyohashi University of Technology researchers led by Associate Professor Shibatomi developed a new catalytic reaction to produce chlorine-containing organic molecules in isomerically pure (left- or right-handed) forms.

Molecules don't have hands as such, but some of them are left- or right-handed. Many chemical compounds display a feature called chirality, where two versions—known as enantiomers—exist for the same molecule. Although their atoms are connected in exactly the same sequence, the two enantiomers are distinct mirror images, like a pair of hands.

Enantiomers can have very different properties. For example, only the right-handed form of glucose gives you energy—the left-handed isomer cannot be metabolized, even though it tastes the same. Many pharmaceuticals are also chiral, and often only one enantiomer has a medicinal use. Therefore, chemists working on complex molecules have developed a variety of tricks to guarantee isomer purity. However, for some reactions this remains a challenge.

Now, the research team has developed a reaction to produce an important class of compounds in pure left- or right-handed form. Organohalides are molecules in which a halogen, such as chlorine, is bonded to carbon. Many are found in nature, or used in medicine. They can be produced from another family of compounds, carboxylic acids, by simply replacing acid with halogen. Unfortunately, if the target compound is chiral, this substitution produces left- and right-handed isomers in equal amounts.

The research team solved this problem by catalyzing the reaction with a catalyst that is itself chiral. Nowadays, catalysts come in a wide range of shapes and sizes — often rivalling the complexity of the actual target molecule. "We screened a diverse array of chiral catalysts, such as Lewis acid, Brønsted acid, and Lewis base catalysts," study lead author Kazutaka Shibatomi says. "Finally, we found an amine that gave us organohalides with up to 98% enantiomeric purity – even though our starting material was a 50/50 mixture."

The chlorinated products, known as chloroketones, are building blocks for more important chiral molecules like pharmaceuticals. Because chlorine is only weakly bonded to carbon, it can be easily substituted by another atom to make a new molecule. Using one of the many compounds produced in enantiomeric purity by their new reaction, the research team synthesized Cathinone, a natural stimulant.

"The substitution proceeds in a simple, classic way," Associate Prof. Shibatomi says. "While chlorine leaves the molecule on one side, the incoming group approaches from the opposite side. The product's chirality just depends on the arrangement of these atoms, so if you begin with a pure enantiomer, you retain that purity. This could open up a whole class of compounds that were previously a major challenge to produce as pure enantiomers."

This work was supported by a Grant-

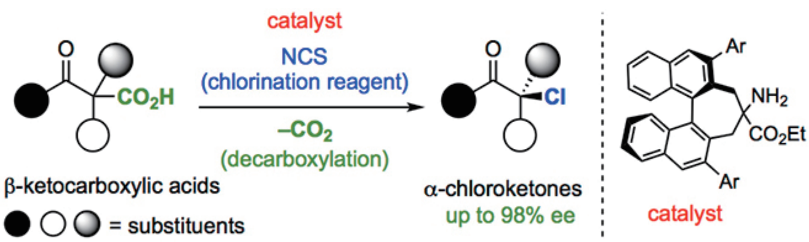


Fig.1 Decarboxylative chlorination of β-keto carboxylic acids.

in-Aid for Scientific Research on Innovative Areas 'Advanced Molecular Transformations by Organocatalysts,' (26105728) and a Grant-in-Aid for Challenging Exploratory Research (16K13993) from MEXT, Japan. Partial support from Daiichi Sankyo Co., Ltd. and Suzuki Memorial Foundation is also acknowledged. K.K. is grateful to the Leading Graduate School Program R03 of MEXT.

Reference

Kazutaka Shibatomi, Kazumasa Kitahara, Nozomi Sasaki, Yohei Kawasaki, Ikuhide Fujisawa & Seiji Iwasa (2017). Enantioselective decarboxylative chlorination of β-ketocarboxylic acids, Nature Communications,
http://dx.doi.org/10.1038/ncomms15600

「らせん型分子接着剤」の発見

－「左巻き」分子は、異なる2種類の「右巻き」分子の「接着剤」として働く－

辻　秀人

辻秀人教授らは、「左巻き」の分子が、異なる化学構造を有する2種類の「右巻き」をくっつける「分子接着剤」として働くことを世界で初めて発見しました。本研究成果は、Nature Publishing Groupの発行するScientific Reportsに2017年3月24日に掲載されました。本研究成果により、従来は組み合わせることが不可能であった、同一方向のらせん構造を有する種々の異なる2種類の高分子を組合せることができるようになり、様々な特性を有する高分子材料の開発を可能にすることが期待されます。

辻秀人教授らの研究グループでは、トウモロコシあるいはジャガイモ由来のデンプンなど、再生可能資源からの生産が可能である「ポリ乳酸」を中心とする「生分解性高分子」に関する基礎および応用研究を行なっています。ポリ乳酸は、代表的な生分解性高分子であり、生体内で加水分解され、分解生成物の乳酸は人体に悪影響を及ぼすことなく代謝されます。このような特性を利用して、組織再生の足場材料など医療用途や環境用途で用いられています。

不斉炭素をもつポリマーであるポリ乳酸には、鏡像関係にあるL体のポリ(L-乳酸)とD体のポリ(D-乳酸)が存在します（図1）。これらをブレンドするとL体どうし、あるいはD体どうしの相互作用よりも、L体とD体の相互作用が強いために、「ステレオコンプレックス」と呼ばれる「共晶」が形成されます。ステレオコンプレックスを形成すると、単独の場合と比較して、融点が上昇し、力学的特性、耐熱性、および耐加水分解性が上昇します。そのため、従来は「生分解性材料」ですが、「ステレオコンプレックス」化により、幅広い用途への展開が可能となります。そのため、近年、ポリ乳酸の「ステレオコンプレックス」化の研究は盛んに行なわれています。

この例のように、ポリ乳酸のL体とD体は、「左巻き」分子と「右巻き」分子の関係にありますので、「左巻き」分子と「右巻き」分子は強く引き合うことを示しています。ポリ乳酸の「メチル基」が「エチル基」に置換された置換型ポリ乳酸の一種であるポリ(2-ヒドロキシ酪酸)（図1）のL体とD体をブレンドすることにより「ステレオコンプレックス」が形成されることも発見していますが、ポリ乳酸の「メチル基」が「イソプロピル基」に置換された置換型ポリ乳酸のポリ(2-ヒドロキシ-3-メチル酪酸)（図1）でも同様の現象が報告されています。さらに同様の現象は分子の側鎖の種類が異なっていても起こり（例えば、ポリ乳酸のL体とポリ(2-ヒドロキシ酪酸)のD体）、これらの結果も「左巻き」分子と「右巻き」分子が強く引き合うことを示しています。

今回の発見は、「左巻き」分子が、従来は組み合うことのない、異なる化学構造を有する2種類の「右巻き」分子をくっつける「接着剤」として働くというものです（図2）。このことは、「右巻き」の分子も、従来は組み合うことのない、異なる化学構造を有する2種類の「左巻き」の分子をくっつける「接着剤」として働くことを意味しています。今回発見した組合わせは、D体のポリ乳酸、L体のポリ(2-ヒドロキシ酪酸)、D体のポリ(2-ヒドロキシ-3-メチル酪酸)です。「左巻き」のらせん構造を有するL体のポリ(2-ヒドロキシ酪酸)が、「右巻き」のらせん構造を有するD体のポリ乳酸およびD体のポリ(2-ヒドロキシ-3-メチル酪酸)をくっつける「らせん型分子接着剤」として働き、通常は共に結晶を作らないD体のポリ乳酸およびD体のポリ(2-ヒドロキシ-3-メチル酪酸)をくっつけ一緒に結晶を作ることを世界で初めて発見しました。本手法を用いることにより、従来は組み合わせることが不可能であった、同一方向のらせん構造を有する種々の異なる2種類の高分子を組合せることができるようになり、様々な特性を有する新しい高分子材料の開発を可能にすることが期待されます。

本研究は以下の助成を受けて行われました。
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- 文部科学省科研費　No. 24108005

見守りロボットのための深層学習を用いた人物姿勢推定

―姿勢推定ビッグデータの効率的生成法―

三浦　純

豊橋技術科学大学の情報･知能工学系　三浦純教授らの研究グループは、人物のさまざまな姿勢を距離データのみから深層学習を用いて推定する方法を開発しました。深層学習では大量の学習データを必要としますが、コンピュータグラフィクス技術とモーションキャプチャ技術を用いて効率的にデータを生成する技術を実現しています。作成したデータは一般に公開しており、広く関連分野の研究の進展に資することを期待しています。

少子高齢化や介護人材不足などを背景に、ロボットによる見守りへの期待が高まっています。例えば、介護施設等での見守りでは、ロボットが施設内を巡回しながら入居者の状態を見て回ることが想定されます。人の状態を知るためには、まず姿勢の推定（立っている、座っている、倒れている等）が有用ですが、これまでの方法は画像を用いるものがほとんどでした。しかし、画像を用いる方法ではプライバシーの問題や暗いところでは適用が難しい、といった課題があります。そこで、研究グループ（平成28年度博士前期課程修了生 西佳一郎および三浦教授）は、距離データのみを用いて姿勢認識を行う手法を開発しました（図1）。

立位や座位など、体の各部位が比較的わかりやすい姿勢に対しては、姿勢を高精度に推定する手法や機器はありますが、見守りでは臥位（横になった状態）やうずくまっている状態などさまざまな姿勢を認識する必要があり、これまで難しい問題でした。近年の深層学習（多段のニューラルネットワークを利用する手法）の進展に伴い、画像を用いて複雑な姿勢の推定を行う手法の開発が進んでいます。深層学習のためには大量の学習データを準備する必要がありますが、画像データの場合には画像から各部位を人が見て特定することは比較的容易で、公開されているデータセットもいくつか存在します。しかし、距離データの場合には部位の境界が見にくく、学習データの作成は簡単ではありません。

そこで、本研究ではコンピュータグラフィクス（CG）技術とモーションキャプチャ技術を組み合わせて大量の学習データを生成する手法を確立しました（図2）。この手法ではまず、さまざまな体型のCGデータを作成します。次にこのデータに各部位の情報（頭部、胴部、右上腕部など11の部位）と、各関節位置を含む骨格情報を付加します。これにより、関節角度を与えるだけでCGモデルに任意の姿勢を取らせることが可能になります。図3にさまざまな座位姿勢に対しデータを生成した例を示します。

開発した手法を用いると、任意の体型の人物と任意の姿勢の組み合わせに対し学習データを生成することができます。現在、座位（隠蔽なし･あり）と臥位のいくつかの姿勢に対し総計10万程度のデータを作成、公開しており、研究目的であれば自由に利用可能です（http://www.aisl.cs.tut.ac.jp/database_HDIBPL.html）。今後はデータ作成のための人物モデルおよびその詳細な構築手順も含めて公開することで誰もが簡単にデータを作成できるようにし、当該分野の発展に貢献できればと考えています。

本研究成果は、平成29年6月3日にPattern Recognition誌上に掲載されました。

本研究の一部は科研費25280093の支援を受けました。

世界初、カルボン酸からハロゲン化合物を不斉合成

柴富　一孝

豊橋技術科学大学の柴富一孝准教授、博士後期課程1年の北原一利さんらの研究グループは、カルボン酸からキラルな塩素化合物を不斉合成することに世界で初めて成功しました。同反応により従来合成が困難であった“キラルクロロケトン”を簡便に高純度で合成することが可能になりました。本研究では生理活性物質合成への応用方法も示されていることから、同手法の医農薬品開発への応用が期待されています。

複雑な構造を有する機能性分子の開発において、これらを精密に合成する技術は不可欠です。中でも医薬品の合成においては、キラル分子の望みとする鏡像異性体のみを高い純度で合成する技術（不斉合成）が必要とされます。生理活性物質の多くは双方の鏡像異性体の薬理活性が異なるため、不要な異性体が混入していると副作用等が懸念されるためです。

キラルハロケトンは医薬品の有用な合成中間体として知られていますが、この化合物を触媒的に不斉合成する手法はほとんど報告されていませんでした。柴富准教授らはカルボン酸をハロゲン原子に変換する脱炭酸的ハロゲン化反応に着目しました。この反応は約150年前に発見された古い反応ですが、これまで同反応の不斉化に成功した例はありませんでした。柴富准教授らは独自に開発した有機分子触媒を利用することでβ－ケトカルボン酸の脱炭酸的塩素化反応が極めて高い不斉収率で進行することを見出しました。本反応では対応するα－クロロケトンが最高98%eeの光学純度で得られます。

得られたクロロケトンの塩素原子は様々な置換基に変換することができます。例えば窒素原子に変換することでアミン化合物が合成でき、硫黄原子に変換すればチオエーテルが合成できます。柴富准教授らは、本手法を利用して強い生理活性を持つ天然有機化合物の合成を達成しました。今後、医薬品の合成ルートの高効率化や新薬開発への応用が期待されています。

本研究は以下の助成を受けて行われました。
- ●科研費　新学術領域研究（有機分子触媒による未来型分子変換）No.26105728
- ●科研費　挑戦的萌芽研究　No.16K13993
- ●博士課程教育リーディングプログラム（超大規模脳情報を高度に技術するブレイン情報アーキテクトの育成）

Pick Up

Special Lecture on "The Minimal Fabrication of Semiconductor Devices and its Social Impact"

On July 4th, 2017, TUT hosted the 2nd lecture meeting of the Chubu chapter of the Engineering Academy of Japan (EAJ).The meeting was held in the newly opened Collaboration Area of the Multi-Plaza in the TUT library.

The EAJ, which is the representative body of the Japan Engineering Society, is composed of leading experts from academia, industry, and government institutions who possess a wide range of knowledge and have made outstanding contributions in engineering and technological sciences, and closely related fields. The EAJ aims to contribute to the advancement of Japan and the world through activities to promote engineering and technological sciences.

At this meeting, two famous Japanese scientists, Dr. Shiro Hara from the National Institute of Advanced Industrial Science and Technology (AIST) and Professor Kazuaki Sawada from TUT, gave lectures on the following topics:

- Dr. S. Hara: The true self of Minimal fabrication technology of semiconductor devices developed by Dr. Hara and its social impact
- Prof. K. Sawada: Recent progress of multimodal sensors developed by Prof. Sawada utilizing minimal fabrication technology.

In addition to academy members from Aichi, Gifu, Yamanashi, Ishikawa, and Toyama, many students and faculty members of TUT attended the meeting.

International Conference of Global Network for Innovative Technology and AWAM International Conference in Civil Engineering - IGNITE-AICCE'17

Toyohashi University of Technology (TUT), in collaboration with Universiti Sains Malaysia (USM), hosted the International Conference of Global Network for Innovative Technology (IGNITE) and AWAM International Conference in Civil Engineering in Parkroyal Penang Resort, Penang, Malaysia between the 8th and 10th of August 2017. Following the success of the previous IGNITE in 2016, USM and TUT once again held the conference in 2017 (IGNITE-AICCE'17) but with a more specific theme of: Sustainable Technology and Practice for Infrastructure and Community Resilience.

Conference Report

The Conference attracted 203 participants including about 100 students and had about 162 oral presentations on 30 sessions covering Structural Engineering, Geomatics/Geotechnical Engineering, Earthquake Engineering, Environmental Engineering, Coastal Engineering, Water Resources Engineering, Transportation/Traffic Engineering, Disaster Management, Sustainable/Green Building Design, Sustainable Development etc.

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Toyohashi University of Technology

The Toyohashi University of Technology (TUT) is one of Japan's most innovative and dynamic science and technology based academic institutes. TUT Research is published to update readers on research at the university.

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