Shimadzu Corporation

Using Artificial Intelligence to analyze mass spectrometer data Automating a highly labor-intensive process

Shimadzu Corporation develops and sells mass spectrometers for analysing pharmaceuticals, food and beverages as well as air, water, soil and others. Analysis of mass spectrometer data is based on identifying the peaks of waveforms in the data. Shimadzu has been working to improve the accuracy of the analysis. Shimadzu commenced research using Artificial Intelligence (AI) in collaboration with Fujitsu Limited and Fujitsu Laboratories Ltd. in 2016. Using AI, the program has sought to automate the 'peak picking*1' process. In order to do this, the partners needed to find ways to generate training data for the system to learn on, and to be able to convert waveform data into images that the system could read.

> *"Fujitsu and Fujitsu Laboratories understand the background of mass spectrometry and responded seriously to our special request. Through this three-way mutual collaboration, we are working to automate the peak picking capabilities of experienced operators."*
>
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Analyzing mass spectrometry data from complex samples is detailed and labor-intensive

Shimadzu Corporation provides products and services globally in a range of fields, including measuring instruments, medical equipment, aeronautical equipment, and industrial equipment. Medical equipment is its largest business segment, accounting for 61% of annual revenue (in fiscal 2016). Shimadzu's high-performance analytical instruments are used for research, technology development, and quality control in many industries.

One such analytical instrument is a high-speed liquid chromatograph mass spectrometer, which is capable of accurately measuring the types and amounts of compound molecules contained in a sample of matter. The instrument ionizes the sample for ultra-high-speed scanning to obtain waveform data, then measures the peak position and height of the waveform data obtained. The accuracy of measurement depends on how precisely the peak can be pinpointed. For this reason, the swift and accurate identification of the peak from complex waveforms has previously been a challenge.

According to Mr. Ryuji Nishimoto "In biological samples like blood, the waveforms are obscured by 'noise' due to the complexity of the substances they contain." To suppress this noise, you need to set hundreds of parameters, many of which could not be handled through the automated settings of the equipment or the dedicated analytical software. Accordingly, experienced operators had to manually identify the peak position by looking at the screen produced by the dedicated analytical software. This was a major burden for researchers and site workers.

Creating training data to enable deep learning to learn

"To address the challenge of processing waveform data" says Ryuji Nishimoto, "we started by talking to Fujitsu, with whom our president already had a long-standing relationship. People working on Fujitsu Human Centric AI Zinrai, which systemizes AI technologies, came to our company, and that's where our joint research began." The idea was to use AI to potentially automate the entire peak picking process. This had been difficult to achieve with equipment and software enhancements, along with all the associated analytical work. Ryuji Nishimoto looks back, "Mass spectrometers are very specialized instruments with limited installations, so we could not easily resolve our challenge by introducing general AI." Shimadzu, Fujitsu, and Fujitsu Laboratories decided to conduct collaborative research, with each company bringing its own expertise in mass spectrometry techniques, equipment knowledge, and AI-based deep learning know-how. The collaborative research began in November 2016. Mr. Shinji Kanazawa (AI Solutions Unit, Technology Research Laboratory, Shimadzu Corporation) served as a leader of the Shimadzu team. He says, "We tried a number of approaches, with each team offering suggestions during discussions on requirements, such as training data needed for deep learning and how to apply deep learning to chemical analysis." Following repeated trial and error, the idea of using AI to resolve the problem began to take shape in June 2017. The Fujitsu and Fujitsu Laboratories teams found that converting the numerical values of measurement results into images and using the data to examine waveform contours were effective ways to achieve the specified accuracy. Meanwhile, the Shimadzu team developed technologies to automatically generate the training data needed to enhance the effectiveness of deep learning. After applying deep learning to more than 30,000 images, they succeeded in increasing the accuracy of peak picking. As of November 2017, work that required around two hours of experienced operator time was achieved in several seconds, thanks to peak picking using AI. Compared with manual peak picking results by an operator with more than 10 years of experience, the automated peak picking results using AI had a false detection rate of 7% and an undetected rate of 9%. By incorporating deep learning into the dedicated analytical software, they succeeded in automatically identifying peak picking with the same accuracy as experienced operators. Also, they managed to smooth out analytical precision discrepancies that occurred with different operators.

Reducing 'peak picking' processes and time Quality enhanced by reproducing the skills of experienced operators

"Fujitsu and Fujitsu Laboratories responded seriously to our special requests," says Ryuji Nishimoto when asked about the reason for the breakthrough outcomes of the collaborative research undertaken by the three companies. Trials are scheduled to begin in June 2018 at the "Osaka University and Shimadzu Analytical Innovation Research Laboratory," established by Shimadzu and Osaka University. Reflecting feedback from this collaborative

research, we expect several dedicated analytical software options to be commercialized and available as early as the spring of 2019. Ryuji Nishimoto concludes, "We hope to work with Fujitsu and Fujitsu Laboratories in the commercialization stages as well." Automation of peak picking is expected to reduce the number of processes and time required for work. It reduces the burden on researchers and site workers, and allows these people to devote their freed time to their own research and development projects. For pharmaceutical manufacturers, incorporating automatic peak picking into the drug discovery process enables them to conduct new drug research more efficiently. The combination of mass spectrometers and automated peak picking is therefore expected to help enrich people's lives.

Customer Profile

Shimadzu Corporation

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*1: The process of reading the width and height of waveforms (peaks) from data acquired by a mass spectrometer