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[Keine Angst vor Künstlicher Intelligenz: KI ist, wenn man's trotzdem macht (vogel.de)]

Machine Learning

No Need to Fear Artificial Intelligence: AI Is When You Do It Anyway

28.05.2022 Guest contribution by Wolfgang Köck, Head of MES & Data Analytics, and Dr. Stefan Pauli, Data Scientist, VTU Engineering

Chemical companies still hesitate when it comes to implementing AI projects. High investment costs, significant effort required and lack of experience – these are the greatest obstacles. Examples from practice show how AI projects can succeed with a 'small steps' policy.

Just 14 per cent of chemical and pharmaceutical companies use artificial intelligence (AI) or machine learning – this was the result of the recent Bitkom study 'Germany learns AI', conducted by the association in 2020. In the Bitkom study the surveyed companies named high investment costs (59 per cent), data protection (50 per cent) and security (46 per cent) requirements and lack of use cases (45 per cent) as the greatest obstacles. The international technology company VTU advocates proceeding in a stepwise manner in data science projects to cautiously approach this innovative branch of computer science. What would such a first step be? What could be a suitable initial AI project? Two data science projects from VTU practice are presented here to provide a better understanding and aid in classification.

Regulating gas pressure with AI

Machine learning was used in a data science project in which a process and its sustainability were optimised in a simple manner. The gas pressure had to be regulated in a process unit. An emergency relief valve was installed to reliably prevent overpressure. The AI-based data analysis contributed to the defining of measures for optimally preventing the opening of the emergency relief valve. It was important for the emergency relief valve to open as infrequently as possible, especially for economic and ecological reasons. Production data from a three-year period were cleaned, combined and used in the analysis. Among other things, the behaviour of the gas flow, gas pressure and valve regulator shortly before and after the opening of the emergency relief valve was investigated. Three typical behaviours were automatically identified and clustered with AI algorithms (k-means).

Data scientists working closely with process technicians were able to identify the three causes of the gas overpressure. After ten days of data analysis, the measures that would reduce the frequency of opening of the emergency relief valve by a factor of four were clear. This greatly reduced not only the amount of process gases lost, but also the air pollution.

Mixture optimization

Another example from VTU practice involves a plant in which a clearly defined mixing ratio – between an expensive and an inexpensive component – had to be maintained. One per cent more of the expensive substance was added to ensure that the dosage was always above the minimum content and thus guarantee the minimum content of this substance at all times. The costs of this one per cent excess dosage added up to several hundred thousand euros a year. Data analysis was used to reduce the fluctuations in the expensive substance content and minimise the excess dosage.

During the data analysis the production and laboratory data from an entire year were cleaned and combined into a data set. Then a machine algorithm for predicting the content of the expensive substance was trained with this data set. This algorithm additionally revealed the parameters that are particularly important for it to be able to make a prediction. This can be very useful when – as in this example – there are about 100 different parameters. Thanks to classic visualisation of the key parameters, new targeted measures that reduced the fluctuations in the substance content and required lower amounts of the expensive substance for the excess dosage could be defined in cooperation with the operator’s process experts. Ultimately, nearly 200,000 euros per year in costs were saved through the result of 20 days of data analysis.

Stepwise procedure for fast entry

These two examples show that even with little effort, great benefit can be achieved with AI algorithms. The stepwise procedure had the advantage of allowing the greatest obstacles to be circumvented because neither high initial investments nor complex data protection measures were required for offline analyses and additionally a use case in the company’s own production arose.

A stepwise procedure with definition of goals, possibly supported by a moderated workshop, in each step has thus proven itself in data analysis projects. After clear and measurable goals are defined, an interdisciplinary team of data science, data engineering, process and/or data security experts is put together according to requirements. Ideally, agile project execution is used to do justice to the exploratory character of the projects. The algorithms are then validated in accordance with GxP, if so required. Finally, the previously defined measurable success criteria are validated and the project success thereby demonstrated in a measurable way for everyone.

Experience has shown that a stepwise procedure offers a low threshold to entry into AI-supported production for all chemical and pharmaceutical companies not yet using AI or machine learning today. It is thus expected that far more than 14 per cent of companies will soon be successfully employing this future-oriented technology.

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Stefan Pauli

Neural networks, machine learning, deep learning, AI – what's the difference between them?

Pauli: It certainly helps to clarify these terms because they are related, but do not refer to the same thing. Elaine Rich's definition from 1983 is appropriate for the general term of artificial intelligence (AI): 'Artificial Intelligence is the study of how to make computers do things at which, at the moment, people are better.' AI thus generally refers to machines that partially artificially emulate human intelligence, that is, partially behave intelligently. Now, there are many different technologies for artificial intelligence. One of them is the machine learning algorithms that independently learn from gathered data. Of these algorithms, there are a few relatively simple ones, such as linear regression or random forest, but there are also very complex ones, such as neural networks. Neural networks combine neurons (nerve cells) in a network, a bit like a human brain with its network of neurons. Large neural networks are then referred to as deep learning, which can demonstrate its abilities very well in image, text or language processing, but requires a large amount of data and computing power. In this way, the hypernym of 'artificial intelligence' leads via multiple intermediate terms such as 'machine learning' to the hyponym of 'deep learning'. What are the key criteria for success on the path from process development to commercialization of a product?

The highly regulated environment and the high risk of failure which accompanies a project to the very end are certainly particular to the pharmaceutical industry. A bad read-out from clinical trials can stop a project on a daily basis, even though everyone is working flat out on it. As in all industries, the key to success is a good product, of course, as well as speed and the associated good risk management, along with a platform which is a well-established as possible.

According to a recent Bitkom study, only 14 per cent of chemical and pharmaceutical companies use AI or machine learning tools. Why is that?

Pauli: AI is already being used by 14 per cent of chemical and pharmaceutical companies. This may sound very low, but the industry average in this study is 13 per cent. Participants in this study were also asked to state the greatest challenges, which shed light on the reasons for the rare use. Large companies stated high investment costs (59 per cent), requirements for data protection (50 per cent) and security (46 per cent) and lack of use cases (45 per cent) as being the greatest challenges. This is in good agreement with our experiences. However, these challenges can be taken into account with an adapted approach. For example, we have had good experiences with a stepwise approach (see next question) in which we start with low investment costs, which only grow later with success. Consistent data protection and security 'by design' can ensure the stability of processes and protect trade secrets and know-how in industrial production.

According to our experience, there is another specific challenge for the chemical and especially the pharmaceutical industry – namely, the strict regulatory requirements and processes. AI algorithms must be GxP-validated. A competent partner with extensive expertise in both worlds, GMP compliance and digitalisation, can provide support here.

From idea to business case: what is the crucial factor for successful implementation of AI projects?

Pauli: Multiple factors come into play here. In our experience, the following have been the most critical:

Identification and definition of a worthwhile and feasible project goal: Some things don't change, not even when AI is used. As with every 'normal' project, the project goals (e. g. SMART) must be identified, elaborated and defined. This can at times be one of the most difficult and most important tasks in an AI project. Guided use case workshops have proven their use here.

Interdisciplinary and experienced project team: Due to the often complex processes in companies in the manufacturing industry, successful project management requires an interdisciplinary team. In it can be found new job profiles such as data scientists and data engineers as well as classic MES engineers and, of course, experienced technicians from engineering and operations, who are very familiar with the production processes. The important thing is to be able to access existing knowledge to make life as easy and successful as possible for the artificial intelligence.

Step-by-step approach: We consider it to be advantageous to develop the projects step by step according to the motto 'Start small and grow with success'. As is the case for other software development projects, the agile project methodology is ideal for this.