

How to implement Machine Learning tools and their benefits in the industry: from R&D data analytics to inline industrial analysis

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Nowadays, Artificial Intelligence and Machine Learning (ML) are gaining tremendous exposure, thanks to many consumer applications (IoT - Internet-of-Things -, smart cities, autonomous vehicles, etc). However, what is the real gain of those Machine Learning tools in the industry in terms of data analytics, such as R&D data analysis or process monitoring?

This paper will show a review of the current Machine Learning tools that can be used to process instrumental data in the industry, from the linear models to the most complex systems such as Artificial Neural Networks (ANN). An extensive comparison of those methods and results will be given on R&D near-infrared (NIR) spectroscopic data ^[1] ^[2].

Those tools can also be implemented inline in the frame of Process Analytical Technology approach (PAT) for process monitoring. Different examples of PAT implementation in the chemical industry will be shown:

- The gain of applying Machine Learning tools for inline product discrimination and chemical composition prediction in a polymerization continuous process^[3] at Arkema production facilities.
- The implementation of Multivariate Statistical Process Control (MSPC) ^[4] for process monitoring within Elkem Silicones company.

[1] S. Roussel, J. Lallemand, S. Preys, 2018. Comparison Machine Learning methods for spectroscopic data analysis. *Vibrational Spectroscopy Group Conference GFSV 2018, Le Ventron, France, 2018*.

[2] A. Croguennoc, J. Lallemand, S. Roussel, 2019; Comparison of Machine Learning methods for spectroscopic data analysis: how to tune Support Vector Machine models for spectroscopic quantitative predictions, *Conférence Chimométrie 2019, Montpellier, France, 2019*.

[3] S. Montagnier, J. Lallemand, P. Hebert, J. Guilment, S. Roussel, 2020. Polymer identification and quantification during continuous in-line processes by near infrared spectroscopy. *Conférence Chimométrie 2020, Liège, Belgique, 2020*.

[4] S. Preys, A. Zenner, F. Gaulier., M. Davezac, 2020. From complex real-world data to process understanding and monitoring, a use case in the chemical industry, *Conférence Chimométrie 2020, Liège, Belgique, 2020*.