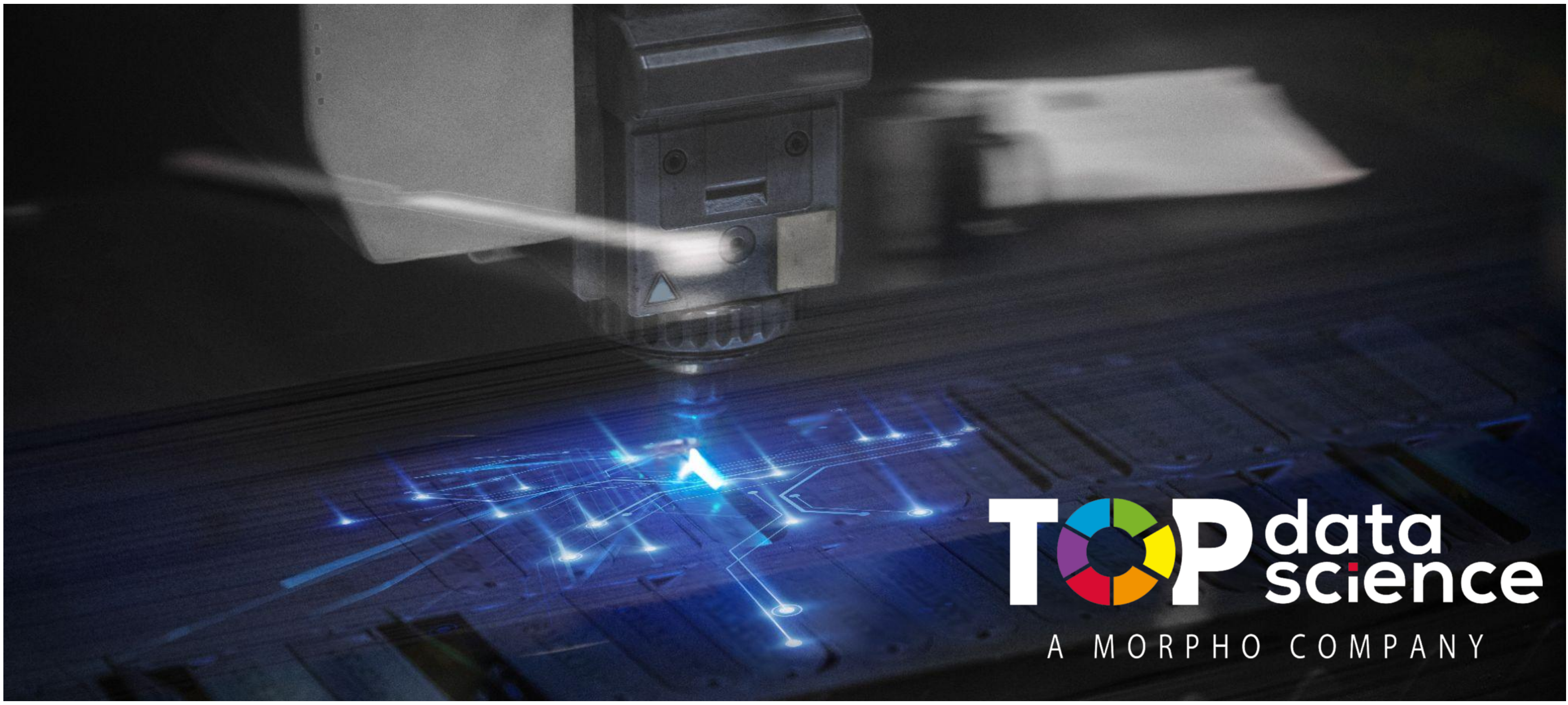


Whitepaper

Artificial Intelligence for IIoT and Process Optimization

The ultimate goal of industrial process control is to improve the plant's performance in terms of uptime, quality and production. Operators of industrial processes want to have the ability to stabilize processes, to predict what will happen in the future, to evaluate alternatives scenarios in processes, and more than these, to have some tools that can recommend the right operative decisions to make.

Executive summary

As a well-established technology for advanced process control (APC) in many industrial applications, model predictive control (MPC), to some extent, has been able to control multivariable processes with complex constraints, with delays and with strong interactive feed-forward and feedback loops. MPC works by intensively reading process variables, feedforward variables from and sending manipulated variables to distributed control systems (DCS) using OPC or OPC UA protocols, to provide setpoints to control processes.

Artificial Intelligence (AI), especially deep learning neural networks (DL), can bring MPC from the traditional rule-based to more data driven mechanisms of controlling, which is a solution to the configuration challenges of traditional MPC implementation. DL can bring some advantages including the ability to learn process complexity such as delays, the flexibility in model construction, the modularity in solution building and the scalability with large datasets.

To be successful with AI for MPC, industrial companies should position AI as a key role in their digital transformation. The key factors are the deep industrial domain knowledge, the readiness of IT infrastructure including data, the state of the art AI toolboxes and world-class AI competences.

Top Data Science has experience in applying AI for process optimization in a wide range of industries such as ***enzyme production***, ***fermentation processes***, ***biofuel production processes***, ***drug manufacturing processes*** or ***pulp bleaching processes***. In the pulp production examples, the quality parameters are properties of the pulp (in different stages of the production line), such as brightness, kappa number (which measures amount of remaining ligning), viscosity and so on. The primary control parameters are the different chemicals used to bleach and adjust pH of the pulp. The secondary control parameters include, among other things, the temperatures and flow speeds at different stages of the process.

Technological Description

AI-based MPC can be simplified as a two-stage approach. In the first stage, models are built to predict what will happen in the process, given the selected ***control parameters*** and ***recent process measurements***. Such models can be learned based on historical data recorded from a system. In the second stage, the models are used to optimize the control parameters so as to steer the system into a desired state. In other words, we use the models to predict what will happen with different control settings, and then find a setting of the controls that gives the desired results.

Methods and Tools

There are many potential modeling techniques that could be considered for constructing the prediction model. The most prominent approach is to use neural networks which provide several advantages.

Key advantages of neural networks

- **Flexible nonlinear** model construction.
- **Easy to build modular solutions.** For example, each stage of the mill is modeled separately, and then these models are combined.
- **Easy to build sequential time series models**, which can for example learn process delays automatically.
- **Scalability to large datasets** (also pretty good scaling in the number of variables).
- **High-quality open source tools** are available, and these libraries are likely to be maintained and developed long into the future. Currently, the adopted library for the modeling toolbox is Pytorch.
- **Automatic differentiation** allows computing gradients of the model prediction with respect to the inputs, which allows also for gradient based control plan optimization.

Even though the neural networks are very flexible and certain model structures perform well across several different applications, there is no guarantee that the same model structure performs well in every single problem. Thus the modeling toolbox should ideally have implementations for several good candidate models, as well as tools for easy model assessment for selecting between different models. Adding new model structures should be effortless.

Another fundamental limitation worth keeping in mind is that MPC requires constructing a ***causal*** model. This is a highly nontrivial task, and very difficult or even impossible to automate completely. Hence the modeling step might involve considerable work from ***domain experts***. This step consists of designing the exact model structure, preprocessing the existing training data, designing what variables are to be predicted and what should be used as inputs, and so on.

Optimization

The MPC framework allows for flexible optimization, depending on the customer's needs. For example, it is easy to impose constraints on the values of the control variables. It is also possible to add penalization that encourages control plans with desired characteristics. For example, we might want to achieve a certain output quality of the bleached pulp but use as small doses of chemicals as possible. In this case we would add a penalization term that penalizes plans with large dosages.

Neural network models are differentiable, so they allow for gradient based optimization of the control plan. In addition, evolutionary or iterative random shooting methods provide a useful alternative for plan optimization. These are often easier to implement, they can be more easily tuned for a specific task, and they typically facilitate inclusion of more complicated optimization constraints (better than gradient based optimization). The current version of the modeling toolbox currently implements one algorithm of this type.

Also with plan optimization, it is evident that a single algorithm will not work ideally in every single application, since different problems will have different characteristics. Thus the modeling toolbox should implement at least a few optimizers, and include the possibility of adding more optimizers easily.

Restrictions, ideas and discussion points

Below there is a list of features or topics that are important to consider using AI and this solution in industrial environments and use-cases.

Continuous control vs. batch processes

By batch process we mean a process that has certain design or control parameters that affect the outcome, but these control variables are not adjusted during the process, but only at the beginning, and then the whole batch is run with this setting. These sorts of problems could naturally be solved using model based optimization (just like MPC), but the difference is the lack of temporal dimension, which might actually make things somewhat easier (batch processes might of course have their own difficulties).

Fully autonomous vs. advisory suggestions to a human operator

This is a crucial question that primarily needs to be decided by each customer organization. A software that could be used to control processes alone, or a system that is meant for advising purposes only?

Real time requirements

Although MPC provides a very generic framework, the implementation details are heavily dependent on the kind of application, especially the real time requirements. For example, optimizing an industrial process is relatively easy, since the delay from control to response in product quality is typically at least minutes or even hours. Therefore one typically has plenty of time for control plan optimization. This is in stark contrast to applications such as autonomous vehicles or other robotics applications, where the control plan optimization typically needs to happen within a fraction of a second. This imposes a lot of constraints on the underlying technology.

How to handle adversarial controls (lack of extrapolation ability)

One well-known problem with MPC is that during the plan optimization, the optimization algorithm might query the model with a control setting that the model has not seen. In this case the model prediction might be substantially off, which might mean that the optimizer will exploit the errors of the model. Especially for autonomous systems, this problem would need to be addressed carefully, and there are approaches for this. For advisory systems this is not as severe of a problem, as we might for example require that the suggested plan cannot be too different from the one a human would choose which will greatly mitigate the problem.

Online learning

Do the models need to support online learning (models updated automatically whenever new data arrives)? This adds quite a bit of complexity. With neural networks it might also be pretty difficult. Our current approach is an approach where we retrain the models on regular intervals.

But even this is not necessarily as easy as it might sound, since neural networks especially are sensitive to the chosen hyperparameters, and the optimal setting might change once the data changes. So hyperparameter validation would be needed. There are challenges on how to reliably make automatic preprocessing of the new data, which would be crucial. Yet an alternative approach would be to just freeze the trained models, and build some system that tracks the performance. If the performance starts to degrade, then the system would figure out why this is the case and only retrain models if needed.

Anomaly detection

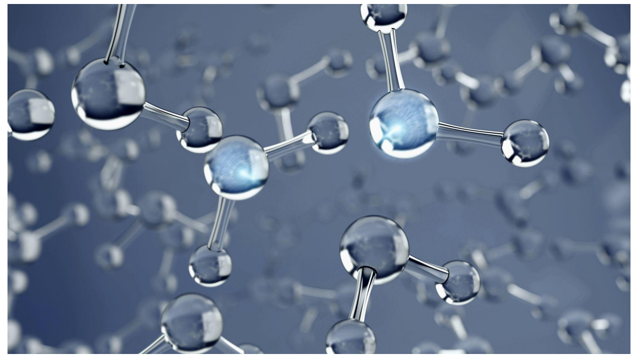
A customer might want to have a system that detects anomalies during the process operation. This essentially means training a model that can recognize when the observations do not look normal with the given control setting (normal meaning something the model has seen so far). This is not very difficult and completely doable, and we can implement it whenever a client indicates interest in such a tool.

Use cases

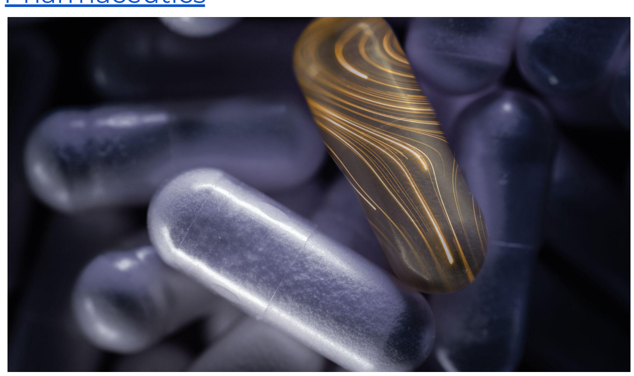
Top Data Science brings our best practices, the state-of-the-art tools and world-class expertises in AI and software engineering to help industrial companies in industrial processes optimization. We have delivered AI applications in a wide range of industries such as pulp bleaching, biomaterial concrete, enzyme production, detergence, biofuel and drug manufacturing processes.

Top Data Science Industrial AI solution for Pulp and Paper is used in multiple production lines and mills. End products, whose quality and production has been optimized using the solution, include dissolving pulp, soft and hard wood pulp as well as fluff pulp. The high-value of the solution, both for the pulp business as well as for the production personnel, has been verified through the close collaboration with StoraEnso.

Digital Detergent Formulation Concept - Top Data Science helped our clients to utilize machine learning to predict the wash performance of washing machine detergent formulations (including enzymes, surfactants, soap, citrate ...), which are targeted given stains in washing setups (temperature, main water, water hardness ...). The clients use such solutions to accelerate their R&D to bring new products to the market faster.



Utilizing Artificial Intelligence in commercial pharmaceutical production to improve the process understanding and eventually the product quality. Top Data Science collaborated with Orion Pharma and University of Helsinki to develop machine learning models to predict Particle Size Distribution and Tensile Strength, two parameters that are controlled to achieve the quality targets of the end-use products. The work is published in [International Journal of Pharmaceutics]



About Top Data Science

A highly experienced team of data scientists, software engineers and business development professionals from Helsinki, Finland.

Excellent customer track record in Finland, Germany, Denmark, Japan, Vietnam, Israel, USA

100+ AI/Machine Learning projects & solutions delivered

AAA® credit rating 2018-2021

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