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Model predictive control of batch processes with Umetrics® Suite of Data Analytics Solutions

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In the pharmaceutical industry, it is becoming increasingly clear that predictive process models and advanced analytics can be of enormous assistance in solving many of the unique challenges. Advanced data analytics tools are used by industry to find the golden nuggets in historical data, aid in process development, fine-tune production, and achieve long-term improvements in product quality and throughput.

Even if one uses highly advanced real-time analytics, they can only analyze what has happened up to the current time point. They are unaware of the problems that will occur further on in the process. The ideal scenario will of course be to have the ability to predict the future of the process and use that information to avoid future problems from happening. If we know and understand the future, we can make changes upfront to improve future results. Figure 1 illustrates an ongoing process highlighting the actual and expected trajectory of the process.

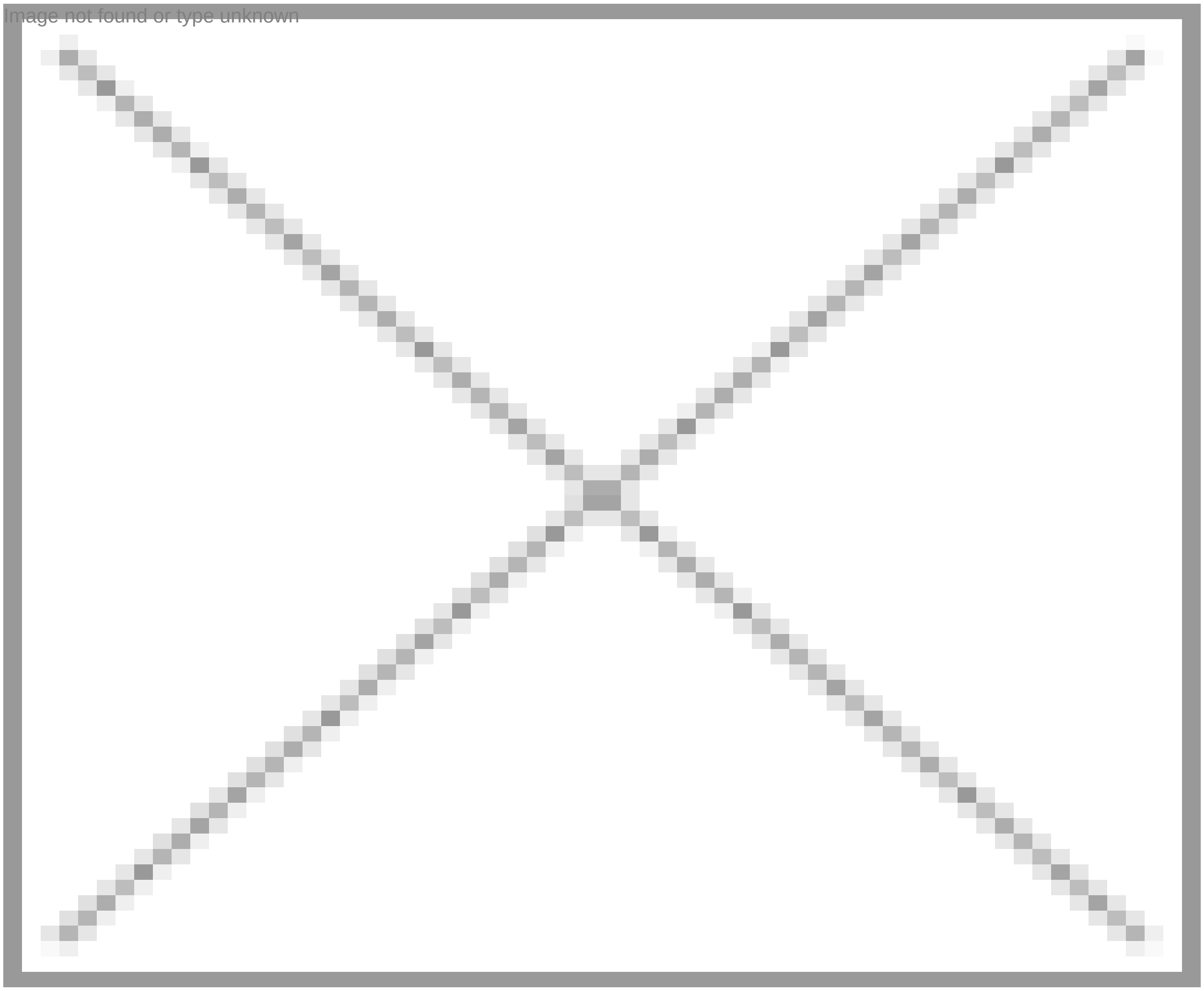

Figure 1: Actual trajectory of a process (black dotted line) & expected trajectory (green line) emphasizing the unknown nature of future trajectory.

How to predict the future

Let us approach this with a simple example, assume there are two process variables- x1 & x2 that are correlated (Figure 2).

Figure 2: Correlated variables, x1 and x2.

If we only measure x1, we can refer to the historic data and plot our estimates onto a scatter plot. We can draw the line of best fit and use it to estimate the likely results of x2 for new measurements of x1 (Figure 3). The method to get these values is called imputation.

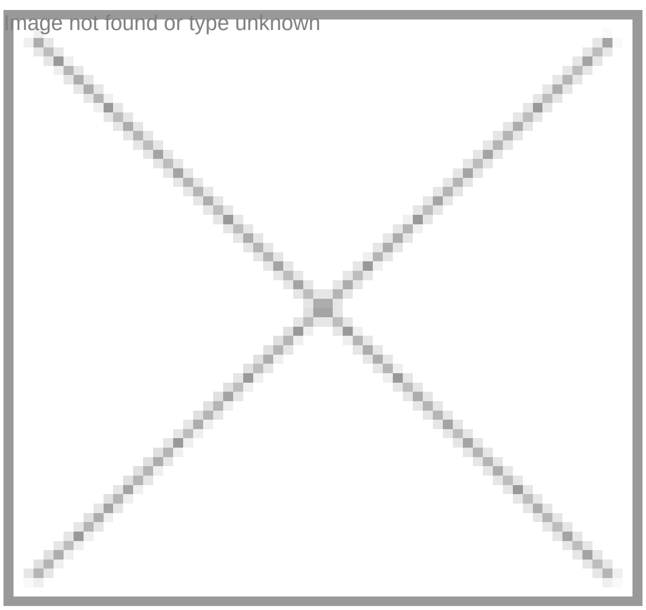

Figure 3: Using correlation to impute the missing value of x2 from x1

In real-world applications, similar estimations of future values of critical process parameters are done using sophisticated missing value imputation algorithms that involve multiple variables at the same time. This is how we arrive at the predicted “open loop” future performance in figure 4.

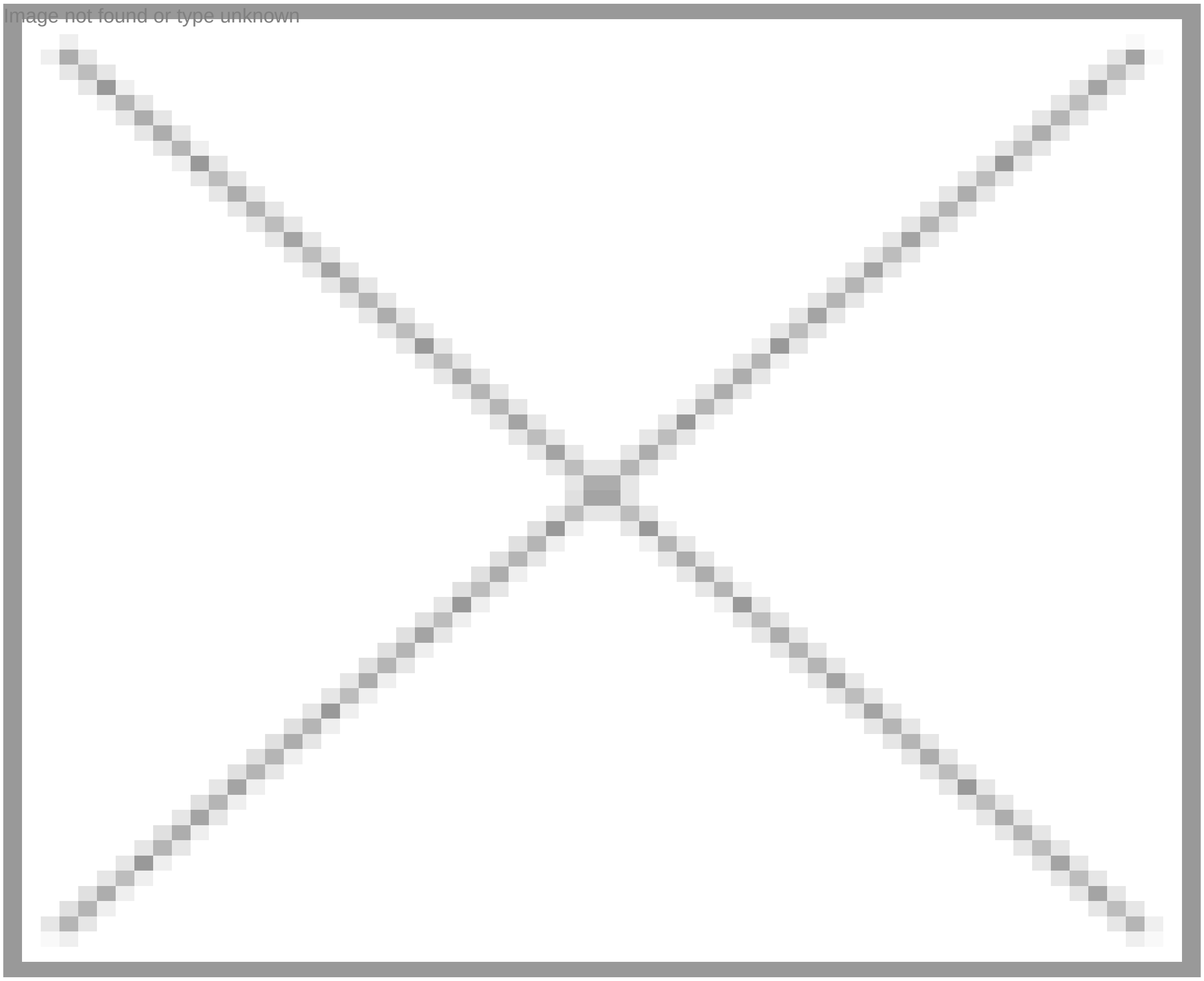

Figure 4: Actual trajectory of a process (black dotted line), expected trajectory (green line) and predicted "open loop" future performance of the rest of the process (blue dotted line).

Model Predictive Control: How to use predictions to optimize performance

Model predictive control or statistical process control is a methodology where one can use predictions to control and optimize a process. The goal is to find the best future settings of your process variables, in order to arrive at the desired outcome of your future process. For example, if you run a biological process, you might collect data for variables such as pH and temperature. Model predictive control can then be used to adjust the future values of the variables, in this case pH and temperature to optimize the future of the process. Umetrics®' SIMCA-online has a powerful tool, Control Advisor, which forecasts and advises future mode for desired outcome.

How Control Advisor works in practice

Control Advisor can be used in both continuous processes and batch type processes. Control Advisor uses existing measurements of the process (up till current time point), future known setpoints and the multivariate model to propose smart adjustments to critical process parameters; this is illustrated in figure 5.

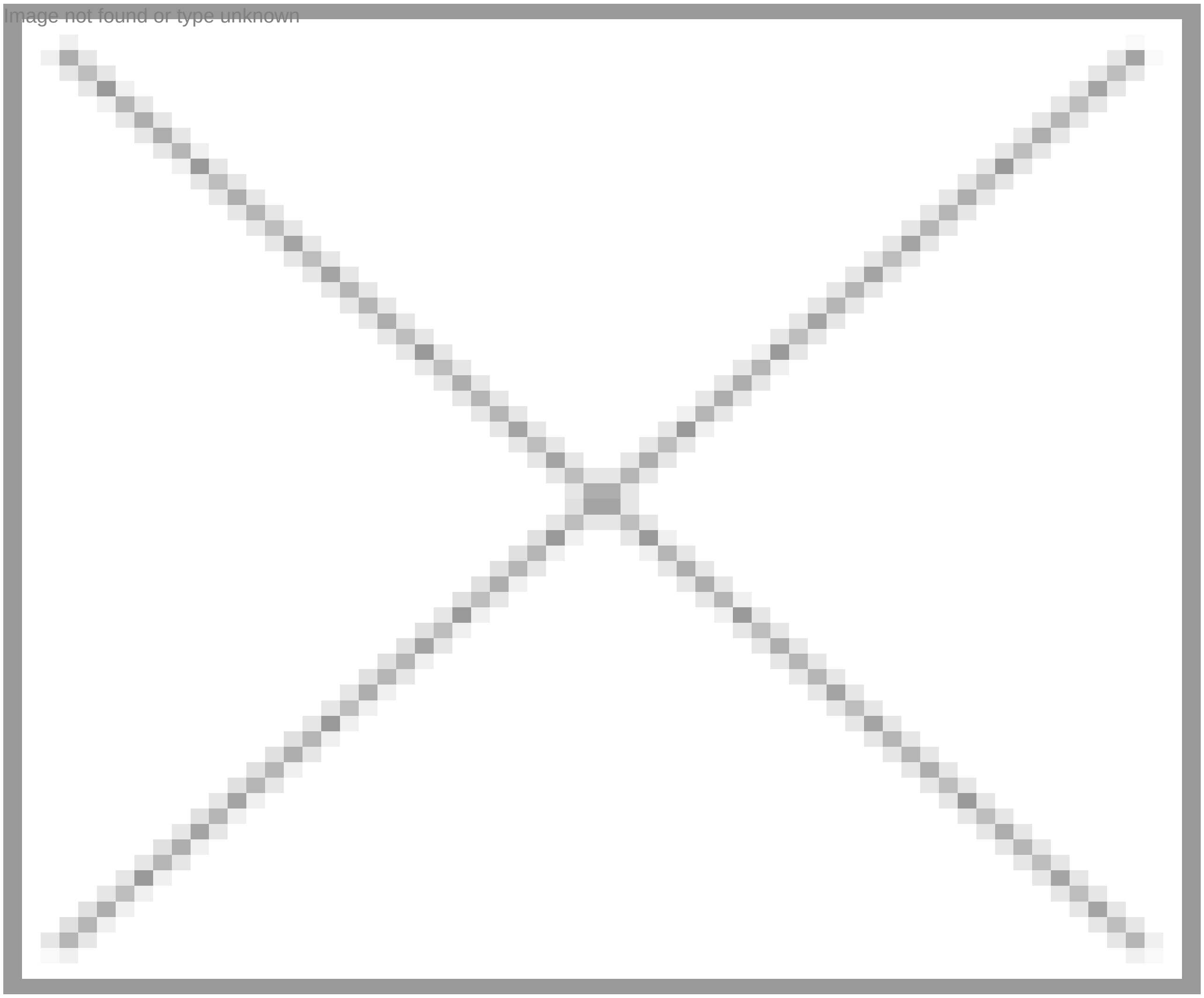

Figure 5: Actual trajectory of a process (black dotted line), expected trajectory (green line), predicted "open loop" future performance of the rest of the process (dark blue dotted line) and predicted "closed loop" future performance following a process intervention as suggested by Control Advisor (light blue dotted line).

Visit www.umetrics.com to download a 30 day free trial of SIMCA-online and use Control Advisor.

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