Bridging the gap between predictive and prescriptive analytics - new optimization methodology needed

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Business analytics is becoming more and more important nowadays. Up to now predictive analytics appears to be much more applied in practice than prescriptive analytics. We argue that although optimization is used to obtain predictive models, and predictive tools are used to forecast parameters in optimization models, still the deep relation between the predictive and prescriptive analytics is neither well understood nor fully exploited. We describe two opportunities to really exploit the synergy between the predictive and prescriptive part. The first is to perform optimization by directly using the predictive models. Adding optimization functionality in predictive analytics tools could be of huge added value for practice. The second opportunity is to replace manual model building with automated data-driven model building, using modern predictive analytics. The pros and cons for such a way of optimization are also discussed.

Key words: predictive; prescriptive; business analytics; data analytics

1. Introduction

1.1. Business Analytics

Business Analytics has become extremely important nowadays. Many companies are looking for Business Analysts and many universities have set up Business Analytics programs, but it seems that at least for the coming years the demand is much higher than the supply (Deloitte 2013). On the other hand, there are warnings that still 'Most organizations have a relatively immature understanding of what 'business analytics' is, let alone how it creates value.' (Stubbs 2016). INFORMS, that also publish the magazine *Analytics*, defines Analytics as follows: 'Analytics is defined as the scientific process of transforming data into insight for making better decisions' (INFORMS 2016). In his famous book (Davenport and Harris 2007), Davenport divides Business Analytics into three parts: descriptive, predictive, and prescriptive analytics. These three 'fields' try to answer the questions 'What is going on?', 'What is going to happen?', 'What is the best action we can take?', respectively.

Up to now, most of the focus in practice is on predictive analytics and the typical methodologies used are data mining, machine learning, forecasting, and simulation. Prescriptive analytics seems to become the next Big Thing (ButlerAnalytics 2014, Lorengan 2015). Gartner's 2014 Hype Cycle for Emerging Technologies predicts that it will still take 5 to 10 years before prescriptive analytics will reach the plateau of productivity (Gartner Inc. 2014). However, what prescriptive analytics is, seems to be unclear, but what can be said for sure is that mathematical optimization is the main methodology used in prescriptive analytics.

1.2. Loose connection between Predictive and Prescriptive Analytics

There seems to be a loose connection between predictive and prescriptive analytics. It is certainly true that optimization is used a lot in predictive analytics to obtain predictive models, as these are typically obtained through minimization of residuals of the models. Moreover, predictive analytics is used a lot to predict parameter values in optimization models, or more recently, to specify confidence intervals for the parameters in order to obtain robust solutions. However, our statement is that the deep relation between predictive and prescriptive analytics is neither understood nor exploited.

We have studied several textbooks on Business Analytics (for example, (Evans 2013, Schniederjans et al. 2014)) and in all of them a completely new topic seems to be started when the prescriptive analytics part begins. For example, many of these books start the prescriptive part with linear optimization, which clearly fits the question 'What is the best action we can take?', but the relation to predictive analytics (typically discussed earlier in the books) is unclear.

Moreover, most optimization experts know little about modern predictive analytics methods and tools. It seems that they are able to apply prescriptive analytics without modern predictive analytics. Several conferences on topics as 'Big Data and Optimization' have been organized, but the works presented there are more about solving large-scale optimization problems in order to obtain predictive models. Optimization certainly can play and does play an important role in obtaining predictive models, but in this paper we argue that there is a more fundamental role for optimization.

This watershed between predictive and prescriptive analytics is also visible when considering the software tools. In predictive analytics tools, although optimization techniques are often available to obtain predictive models, the prescriptive analytics techniques are not implemented. On the other hand, although optimization software companies use the term 'prescriptive analytics' to promote their software, the connection to predictive analytics is not exploited. As far as we know, RapidMiner (RapidMiner 2016), one of the most used predictive analytics tools, starts to realize the added value of prescriptive analytics (Mierswa 2014).

We discuss two opportunities for optimization to enable a fruitful connection between predictive and prescriptive analytics. First we describe that there is much added value when optimization is carried out together with predictive models. Such optimization could be added to the predictive analytics tools. This opportunity is discussed in Section 2. The second opportunity directly concerns the way of working in the optimization field. For some of the optimization applications we plea to generate the models via a data-driven predictive analytics methodology instead of doing manual model building. This opportunity is discussed in Section 3. The first opportunity is about how optimization can give added value in the predictive analytics field, whereas the second opportunity is about how predictive analytics can be beneficial for model building in the optimization field. We also show that these two opportunities ask for a new optimization methodology.

1.3. Literature

In the predictive analytics world there is much confusion about prescriptive analytics. The difference between predictive and prescriptive is often not well understood. In (Vorhies 2014) this distinction is even questioned by using the argument that the predictive analytics results already directly imply the best actions to take. Although not using the words predictive and prescriptive analytics, in his presentation Andrea Lodi (Lodi 2016) suggests that Machine Learning and Optimization should be more integrated. Simchi-Levi (Simchi-Levi 2014) discusses the importance of data-driven modelling: instead of using data to feed the model, use the data to obtain the right model.

In the most advanced work on this topic we found so far, Bertsimas and Kallus (2014) combine machine learning techniques and optimization to integrate predictive techniques for uncertain parameters and manually built prescriptive models, instead of just using predictive analytics to predict uncertain parameter values as input for prescriptive models. In relation to the second opportunity discussed in this paper, we propose to go even further by integrating predictive analytics and optimization to obtain automatically built prescriptive models.

2. Optimization with predictive models

2.1. Extra functionality in predictive models

To really fulfill the Business Analytics promises of 'smarter decisions, better results' (Davenport et al. 2010), we advocate to add optimization technology directly to the predictive analytics techniques and tools. When predictive models are generated that predict the outcomes and the corresponding uncertainties, then one can use the optimization power to search for the best action that satisfies all the constraints and maximizes the objective value, thereby taking into account all uncertainties detected by predictive analytics.

Let us describe our proposal in more detail, by describing how optimization could be added to predictive analytics tools. To just illustrate the essence, we describe a basic, simple format; in Appendix A we discuss a more general one. Consider a general application implemented in a predictive analytics tool, in which $x_1, \ldots, x_n$ are the input variables, and $y_1, \ldots, y_n$ are the output variables. The user feeds the tool with data on x and y, and specifies the bounds on the optimization variable x and on the output factors y, and specifies one of the output variables y_i as objective function. Next, the user presses the button 'optimize' and the tool develops predictive models for $y_1, \ldots, y_m$ (in relation to the past data on x) and uses the optimization technology to find the best values for $x_1, \ldots, x_n$. Hence, although the tool uses predictive analytics to obtain the models, for the user there is a direct connection from data to optimization.

2.2. New optimization methodology needed

Technically speaking, using all kinds of predictive models leads to general mixed integer nonlinear optimization (MINO) problems, which cannot be assumed to be convex. Moreover, since almost always (model) uncertainty would play a significant role, the optimization method should be capable of dealing with such uncertainties. Robust Optimization (RO) and/or Stochastic Programming (SP) could be used for this. Although the MINO, RO and SP fields have shown impressive progress in recent years, the combination of mixed integer, nonlinear, nonconvex, and stochastic parameters remains a big optimization challenge. The trade-off between model accuracy and computational complexity for optimization is an important issue here.

Furthermore, optimization methods that exploit the special structure of the predictive models could be developed. It is possible that adapted and extended versions of Ordinal Optimization (Ho et al. 2008) or Ranking and Selection (Boesel et al. 2003) could appear to be efficient.

2.3. Relation to existing approaches

In this section we briefly discuss the relation of the proposed approach to the well-known existing optimization approaches – model predictive control and black-box optimization:

- Model predictive control (MPC, see e.g. Camacho and Alba (2013)) is an approach to control processes in which at each stage, a limited-horizon version of the control problem is solved and the optimal here-and-now decision is implemented. In later stages, this procedure is repeated.

Repeating our predictive-prescriptive approach over time, it may resemble that of MPC. The difference, however, lies in the model construction. Whereas in the MPC it is simply a finite-time version of the known model of the control process, with the same functional form but different (estimated) parameters, the proposed approach allows for a different predictive-prescriptive model at each stage. Since the past information on the MPC input and output is used, one can speak here of learning the model in time.

Another angle from which it may seem that there is a close connection between the MPC and the proposed approach is the necessity to deal with uncertainty about the model shape. However, the variants of MPC in which uncertainty is taken into account, such as the tube-based MPC (Mayne et al. 2011) or min-max MPC (Martino Raimondo et al. 2008), rely on a full specification of the model itself and handle parameter uncertainty. In the proposed approach, the uncertainty relates to the entire relationship between the input and the output.

- Black box optimization (see, e.g., Scheinberg et al. (2009), Cassioli and Schoen (2013)) is a paradigm where one minimizes a function for which only limited information is provided by an oracle at a given point (e.g., value, finiteness, gradient) chosen by the decision maker and the oracle may be expensive in terms of time or money.

Our proposal could be seen as a special case of black-box optimization, but with a different exploration-exploitation trade-off than in problems considered commonly. In standard black-box, there is little data available and one gains more information through *exploration* - investigating new possible solutions. This information is then *exploited* to find the best solution. In our setting, on the other hand, there is already a lot of data available on the function value at certain points that can be exploited and the initial balance is skewed towards exploitation. Whereas in some settings it might not be possible to gain more information through exploration, in other situations exploration may be a part of the optimal strategy if learning effect is taken into account, for example, in a multi-armed bandit-type problem.

3. Automated, data-driven instead of manual optimization model building

3.1. Classical model building

One of the first steps in mathematical optimization is building the model. After identifying the key issues in a certain decision problem, both the objective and the constraints are formulated in mathematical terms. The art is to keep the model as simple as possible, but such that it still contains the most essential aspects. Examples of optimization models are linear, second-order-cone, semi-definite optimization models. This manual model building process has the following disadvantages:

- It has to be done by an optimization expert, someone who is trained in optimization and in complex situations model building is an art (Baker 2015).
- It normally costs a lot of time before all processes are understood, and to build a model that captures all relevant issues. For this reason, the model builder can only analyze a few alternative models.
- The problem setting normally changes rapidly, e.g., new types of constraints have to be added for an optimization expert is needed again to re-build the model. Moreover, the change may require a (totally) different optimization model, see e.g. the *concept drift* issue (Van Leeuwen and Siebes 2008). An even more dangerous situation may occur when the change in problem environment is not observed, and the model is not valid anymore.

- Often the objective and/or constraint functions are surrogate functions, i.e., they do not model reality directly. As an example we mention the penalty objective function in Intensity-Modulated Radiation Therapy (IMRT) – this function penalizes deviations from a target dose. However, this function does not model the real effect on tumor and healthy organs.
- It is not data-driven – in fact, in the classical optimization approach first the model is built and then it is fed with the required data (Bisschop 2016).

3.2. Automated, data-driven model building

Instead of manual model building we advocate to consider the opportunity to simply start from the data, and use modern predictive analytics to define all constraints and objectives for the optimization process. Hence, constraints or objective functions could be formulated by e.g. machine learning models, support vector machines or symbolic regression models.

We realize that this approach also has disadvantages and it may not be feasible for many applications, which will be discussed later in this paper. However, for applications that significantly suffer from one or more of the disadvantages of manual model-building mentioned in Section 3.1, such a predictive analytics way of obtaining the model might be beneficial (for example, engineering systems that are too complex to model manually). Moreover, we think that in practice a combination of manual and automated data-driven modeling could often be used. Predictive data mining and/or process mining (Van der Aalst 2016) techniques can be used to model those constraints or objectives that are 'hidden' and that are difficult to model manually without data.

3.3. New optimization methodology

Of course, this way of model building also leads to different types of optimization problems. Hence, the same new optimization methods as described in Section 2.2 are needed here.

The opportunity just described requires a new way of model building. In the classical optimization approach the following steps are advocated in this order: problem investigation, model building, data gathering, model validation, model solving, sensitivity analysis, decision advice. The approach we advocate is to switch the order of 'model building' and 'data gathering', possibly merging the two, as illustrated in Figure 1. This data-driven modeling idea is not new, but our proposal to use modern predictive analytics to find (part of) the model goes even further. As advantages of such a way of model building we can just mention the opposite of the disadvantages of the manual model building discussed in Section 3.1. As an example we take the last one: with automated model building one can evaluate thousands of different models, and take the best one. As an extra advantage we mention that the step 'model validation' is automatically included in

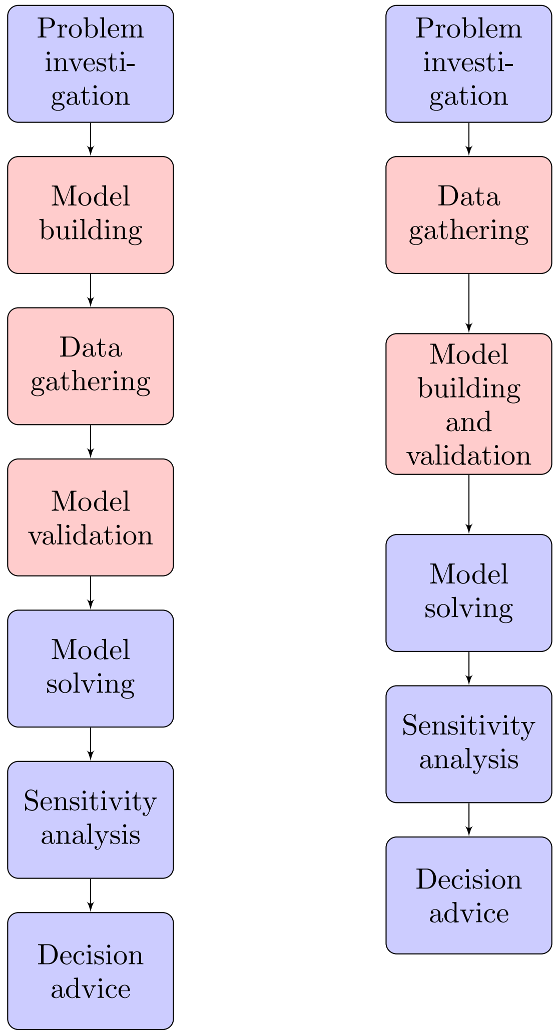

Figure 1 Comparison of the classical model building (left) and the new approach (right).

our approach, while in the classical approach this step is often neglected since it costs too much time.

In the context of Robust Optimization, where prediction accuracy is important, we expect that this could also lead to the development of new predictive models. For example, it is important to have high prediction accuracy in all kinds of robust models related to structures with safety constraints, as met in complex engineering applications.

3.4. Examples

In this section we present several practical examples in which the classical model building suffers from certain difficulties and where the proposed approach could be seen as a viable alternative.

- **Waste water treatment plant with pump stations.** A waste water system consists of a waste water plant that cleans the water, and a number of pump stations that pump the waste water from the storage to the plant. The problem is to find an optimal pump strategy such that the total amount of water per time unit delivered at the plant is as constant as possible, and also such that the amount of water in the storages remain between specified lower and upper limits. (Yamaner 2014) developed a linear optimization model, for which some simplifying assumptions on the physics had to be made.

In the approach described in this paper, we would use data from the past on the weather predictions, real precipitation, pump strategy, storage levels, and inflow at the plant. Based on this data one could develop a predictive model that predicts the inflow at the plant for a certain pump strategy. This model could be used to optimize the pump strategy.

- **Personalized cancer treatment optimization.** Optimization is used nowadays to optimize the radiotherapy treatment plan for a patient with cancer. The optimization model that is used contains of course patient data, but this model is based on theoretical (biological) considerations (see Hoffmann (2013)).

In the approach we advocate, we would use data of a huge number of patients treated for the same type of cancer. The data contains not only a characterization of the tumor, the implemented treatment plan, and the medical results of the treatment, but also data on e.g. weight, gender, and age of the patient. Predictive models are developed that predict the medical outcome if a certain treatment plan is used for a specific patient. Using this predictive model, one can optimize the treatment plan for this patient.

- **Traffic light optimization.** Consider a traffic intersection with many lanes that is controlled by traffic lights. Models based on e.g. queueing theory have been developed, which are used in practice to find optimal green / red times for each lane (see Nellore and Hancke (2016)). Given the current traffic intensity at each lane, the average waiting time is minimized. Although the prescriptive model that is used is fed with data, the model itself is based on theoretical considerations and is not data-driven.

In the approach we suggest in this paper, we do not use the (queueing) model, but we use the data from the past to generate a fully data-driven predictive model. Hence, the historical data on traffic intensities, green / red times, waiting times, etc. is used to generate a predictive model that predicts the average waiting time for a specific traffic intensity and green / red time profile. This automatically generated (and constantly updated) model is used to calculate the optimal green / red time profile for the current traffic intensities.

- **Distribution of new cars.** This is an example where only a part of the model is generated automatically. Consider the distribution of cars of different types and length. It appears to be very difficult and time consuming to derive manually a model that predicts whether a set of certain types of cars will fit on a certain trailer (the lengths of the cars are certainly not enough to know).

Based on historical data on sets of cars transported by this type of trailer, one could develop a predictive model that predicts whether a certain set of cars would fit on the trailer. This predictive model could be used in a prescriptive model that optimizes the car distribution.

3.5. Possible drawbacks

In this section we discuss several drawbacks or arguments that could be used against the proposed approach.

- **Black-box approach.** The most obvious drawback of the proposed approach is the difficulty of interpreting the model built using predictive analytics tools. Indeed, by the very fact of constructing a model in this way one resigns from understanding the exact relationships between different variables. One can imagine that this can be of problem, e.g., in the radiotherapy application proposed above, as intuitively any kind of treatment of a living person should rely only on a full understanding of the model at hand for safety reasons. In our opinion however, this drawback is not critical in long term as long as the main objective is to find the best decision variable value — in fact, in many areas we already rely on devices or algorithms whose details of functioning we do not understand. Additionally, it may turn out that analytics may provide surprising insights that would be otherwise blurred by a complex optimization model.

- **Computationally more complex.** If prescriptive analytics is considered as an additional tool to a predictive model, it should be noted that not each of such models can be considered as computationally tractable from the optimization point of view. For automated model building, the need to search the space of possible predictive models involves the following as some of the main challenges: (i) which variables to take into account; (ii) what functional form should the model take. All of this involves a huge search space including many integer decisions and theoretically infinite number of possible models and this relates more or less to all four applications proposed above. In fact, it is hard to imagine the methodology without (i) substantial limitations of the model search space, and/or (ii) substantial number of heuristics included. Nevertheless, it should be noted that what is sought is not the optimal model, but a model that yields better decisions faster than the manual model-building and it is possible that already relatively simple models are good enough, especially when the time/objective value trade-off is considered.

- **May need huge data.** It can be expected that building a reasonable model of a (business) process using analytics may require large amounts of data sufficient to reach sufficient accuracy. This can be an issue in applications such as cancer treatment where the size of the images involved is very large or the wastewater treatment where the model at hand is essentially continuous-time before its discretization. Whereas there are applications in which obtaining vast amounts of data is relatively easy — for example, large retailers, energy suppliers, machine learning — it may also happen that not much data is available e.g. due to low frequency of model planning or due to the fact that the business process at hand has a short history. In such situations, traditional model building seems to be the only possible approach.

4. Miscellaneous topics

In this section we discuss several different issues that are related to our proposal.

Little vs. big data. We emphasize that the proposed interaction between predictive and prescriptive analytics in this paper is not only applicable when big data is available. Also in some cases where only 'little data' is available one could generate predictive models and on top of that optimization tools. Of course for such cases other predictive models, such as Kriging models (Krige 1951), might be much more efficient.

Use of process mining in model building. Often in manual model building it takes much time to fully understand the relevant processes. Moreover, it is not unlikely that there is a mismatch between what the experts think the processes are and how they are in reality. For this purpose modern process mining techniques and tools can be used. They use log files to generate a clear picture of how the processes look like in practice which may save time and lead to a better description of the real processes (Van der Aalst 2016).

Better definition of and distinction between predictive and prescriptive analytics. In Section 1.3 we argue that prescriptive analytics is not well defined in the literature, which even led to questioning the added value of prescriptive analytics. Indeed, prescriptive analytics is about making predictive analytics result implementable, by finding optimal decisions. However, in several applications the best action to take follows automatically from the predictive analytics results. Hence, it is important to stress that prescriptive analytics is also about finding the best feasible decision out of a huge number of possible decisions, considering a huge number of possible realizations of uncertain parameters. This optimization task cannot be done by human beings; powerful optimization techniques are needed to perform this fight against the curse of dimensionality. In predictive analytics often Big Data is a challenge, in prescriptive analytics the challenge is Big Search Space.

Prescriptive analytics technology added to predictive analytics tools. Although prescriptive analytics is now more and more seen as the next Big Thing, still a majority of the companies that use predictive analytics are not using prescriptive analytics (Van Rijmenam 2014). For a successful dissemination of prescriptive analytics, we think it is extremely important that the optimization technology is added to and built on the popular and widely used predictive analytics tools. Moreover, the language and the framework should be closely connected to the predictive analytics one. In Appendix A we give a proposal for such a generic prescriptive analytics framework.

Textbooks on business analytics should be changed. From a didactic point of view, we advocate to change the textbooks on Business Analytics. Instead of describing predictive and prescriptive analytics as two separate fields, we advocate to start the prescriptive part by using the predictive models to derive optimal decisions. This means, e.g., that the prescriptive analytics part should not start with linear optimization, but directly with general nonlinear and nonconvex optimization using the predictive models.

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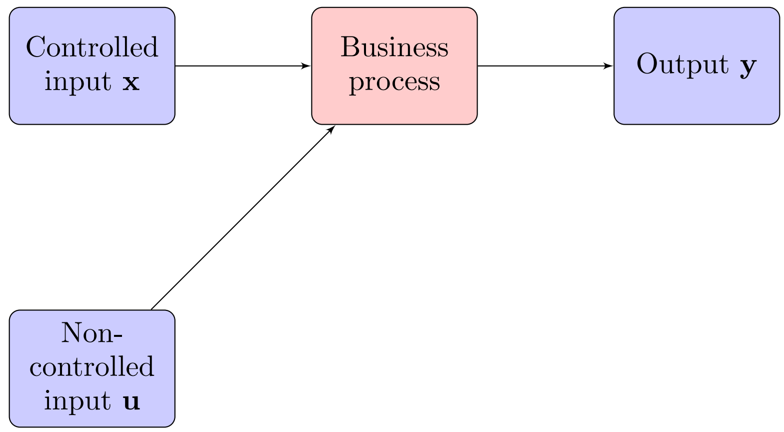

Figure 2 Business process scheme.

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Appendix A: Prescriptive component for a predictive model

In this appendix we present a more technical description of a prescriptive analytics component that could be added to predictive analytics software. This description is still very basic so that the main message can be applied to many existing predictive analytics tools.

For the setup, let $\mathbf{x} = (x_1, \ldots, x_{n_x})$ be the vector of user-controlled input quantities, $\mathbf{u} = (u_1, \ldots, u_{n_u})$ be the vector of input quantities not controlled by the user and $\mathbf{y} = (y_1, \ldots, y_{n_y})$ denotes the vector of output quantities. In this setting, there is uncertainty w.r.t. the future values of the uncontrolled vector $\mathbf{u}$ and the relationship between $(\mathbf{x}, \mathbf{u})$ and $\mathbf{y}$.

For example, in the context of an inventory management problem, $\mathbf{x}$ may correspond to ordering quantities and prices, $\mathbf{u}$ is the uncertain customer demand and $\mathbf{y}$ is a vector corresponding to the level or profit and amount of inventory left. The scheme of a business input-output process is illustrated in Figure 2.

In the predictive analytics approach, the middle term — the business process — is not known exactly, but past information on m observations of $(\mathbf{x}^i, \mathbf{u}^i, \mathbf{y}^i)$, $i = 1, \ldots, m$ is available. Among

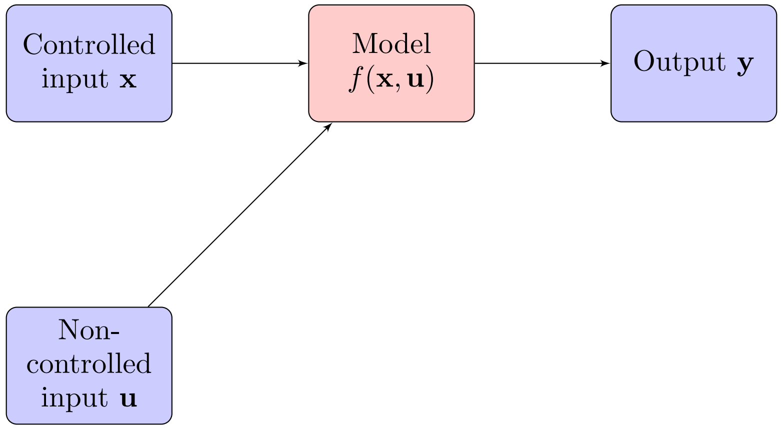

Figure 3 Predictive analytics model of a business process.

many possible predictive models $F_i : \mathbb{R}^{n_x} \times \mathbb{R}^{n_u} \to \mathbb{R}^{n_y}$ where $F \in \mathcal{F}$ where $\mathcal{F}$ is a certain function class (for example, linear or quadratic), the 'best' model F is chosen. This is illustrated in Figure 3.

The class of models $\mathcal{F}$ might be required to satisfy certain *objective function constraints*, related to the properties of the problem. For example, a model that models a traffic system should not provide, for any value of the uncertain number $\mathbf{u}$ of pedestrians and cars, average waiting times $\mathbf{x}$ that would negative.

Typically, the criterion for choosing the model F is to minimize a loss function $L(\cdot)$ over all the observations:

$$F \leftarrow \min_{F \in \mathcal{F}} \sum_{i=1}^{m} L(F(\mathbf{x}^i, \mathbf{y}^i) - \mathbf{y}^i).$$

For example, a common choice is to use the squared loss:

$$\sum_{i=1}^{m} L(F(\mathbf{x}^i, \mathbf{y}^i) - \mathbf{y}^i) := \sum_{i=1}^{m} \left(F(\mathbf{x}^i, \mathbf{y}^i) - \mathbf{y}^i\right)^2.$$

Once a satisfactory model F is found, decision $\mathbf{x}$ is chosen so as to minimize (minimization is a convention here, it can also be a maximization) the maximum value of some function $F(\mathbf{x}, \cdot)$ over the possible realizations of uncertain input variable $\mathbf{u}$

$$\mathbf{x} \leftarrow \min_{\mathbf{x} \in \mathcal{X}} G(\{F(\mathbf{x}, \mathbf{u})\}), \tag{1}$$

where $\mathcal{X}$ is the set of allowed decision variable values. This set might model certain *decision variable constraints*, such as nonnegativity of the amounts of materials or upper bounds on inventory levels.

For example, if one is concerned with the worst-possible realization of $\mathbf{u}$, then the problem solved after clicking the 'optimize' button is:

$$\mathbf{x} \leftarrow \min_{\mathbf{x} \in \mathcal{X}} \sup_{\mathbf{u}} F(\mathbf{x}, \mathbf{u}),$$

i.e. one chooses the $\mathbf{x}$ that minimizes the worst-possible outcome of the model function $\mathbf{u}$.

It is also possible, after choosing the model F, to construct a separate model that estimates the 'most likely' value of $\mathbf{u}$ and insert it as the only possible value of $\mathbf{u}$ in formulation (1).

In this way, the prescriptive part can be seen as another functionality added to the predictive model. Having the need to optimize over $\mathbf{x}$, a preference might be given to models F in which this task is easier to obtain, i.e., there is a need to trade-off the fit of the model F understood as the loss function value, and F's complexity to optimize it over $\mathbf{x}$.

From the scheme presented above, it is clear that adding a prescriptive functionality can be obtained by simply extending the existing predictive analytics tools. Existing analytics tools allow the user to choose from a variety of models and the optimization complexity of each of them can easily be pre-established using certain hierarchical rules. In this way, one can reduce the space of predictive models to the ones with low enough optimization complexity.