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An Ontology-Driven Approach to Improve Data Understanding for Machine Learning Applications in Manufacturing

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Abstract: The application of Machine Learning (ML) methods represents a significant aspect in the advancement of Industry 4.0. The creation of an appropriate data set for these applications has been identified as the most time-consuming step in the underlying end-to-end pipeline. One of the major obstacles in this process step is to bridge the gap between business understanding and data understanding. To address this challenge, we propose a novel methodology to bridge this gap based on a systematic literature review. Our methodology begins with the construction of an ontology that depicts the underlying manufacturing process along with its parameters. We then show how this ontology can be utilized to deepen the understanding of the manufacturing process. Subsequently, we demonstrate how appropriate target variables for ML-models and suitable data sources can be determined with the support of our ontology. We further elucidate our methodology through a real-world example.

Keywords: data acquisition; knowledge graph; Machine Learning (ML); manufacturing; ontology

1 INTRODUCTION

Taking up to 70% of the entire time, data preparation is the most time-consuming step in an end-to-end Machine Learning pipeline [1]. In this publication, we tackle one of the key challenges when it comes to the task of data preparation: bridging the gap between business understanding and data understanding. To this end, we propose a methodology which supports the determination of appropriate target variables and corresponding data sources before setting up a suitable data pipeline. In addition, it provides a depiction of the underlying process which is suitable for exploratory knowledge discovery.

At the beginning, we define six questions one may ask when faced with the task of describing a manufacturing process, with the goal to identifying the target variables and respective data sources needed for the ML-models under consideration. These questions are:

1) What does the manufacturing process look like, i.e. what are the general steps of the process?
2) Which machines are used throughout the process?
3) What happens during the process, i.e. which materials are used in which way to manufacture the final product?
4) What are the attributes or parameters of the various components of the manufacturing process?
5) How are these attributes or parameters related?
6) How to obtain a potential dataset for these parameters?

To answer these questions, we utilize a predefined ontology to depict the respective manufacturing process. This process depiction includes all machines and materials that are used during the process as well as all parameters and their relationship to each other. The general idea is to follow a structured procedure that builds the description of the respective manufacturing process step by step. With an ontology being "a formal, explicit specification of a shared conceptualization" [2] it essentially enables knowledge-based applications by two benefits: (1) sharing and reusing knowledge, which is formally described using a standardized language, and (2) inferring implicit knowledge from explicitly given axioms and facts, based on its formal semantics. Ontologies that primarily focus on particular elements and their relations are often called knowledge graphs.

For us, this means that we only have to define the direct relationships between the respective elements (i.e. machines, materials, or parameters). Implicit relationships are automatically inferred by ontology reasoning using the formal semantics and the logical axioms that we defined about the relationships in a manufacturing process.

We conducted a systematic literature review using the Scopus search database. We used three queries that observed the abstract, title, and key words to search for relevant publications. Our search queries included the terms "manufacturing" and "machine learning" as well as "data acquisition", "feature engineering", and "data source" respectively. In total, we found 488 publications of which we will discuss five in detail that address bridging the gap between business understanding, i.e. domain knowledge, and data understanding. The systematic procedure we followed is summarized in Fig. 1.

In [3], the authors present a methodology for selecting suitable data sources based on a House of Quality matrix. However, the methodology proposed in [3] does not include a depiction of the manufacturing process itself and assumes that a preselection of suitable data sources is already given. In [4], the authors propose a methodology based on a matrix they developed called "ML-SIPOC". This methodology includes a description of the manufacturing process, although less detailed than ours. The main difference to our approach is the utilization of the reasoner, which results in us not having to do the entire reasoning about which data sources may be relevant. Furthermore, the main tools used in the methodology in [4] are the already mentioned ML-SIPOC matrix and flowcharts. These tools do not allow the same level of exploratory and interactive knowledge discovery about the manufacturing process and its parameters as our approach using Web Ontology Language (OWL) ontologies.

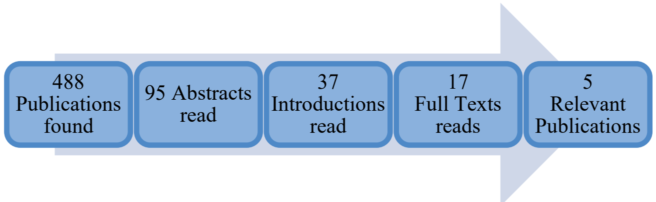

Figure 1 Summary of our literature research

In [5], the authors create an ontology to describe the features of a manufacturing process and use the resulting Resource Description Framework (RDF) graph to analytically compute the similarity of features using graph kernel functions. However, this approach is only used to enhance linear regression models and not generalized. In addition to the utilization of the RDF-graph the authors also present how the ontology they created can be used for feature preselection. This preselection depends on the relationships of the features in the proposed ontology. In comparison, we propose a more detailed description of the relationships between parameters, allowing for more sophisticated applications.

Finally, in [6,7], the authors present different ontologies with the goal of automating as much of the end-to-end ML-pipeline as possible. To this end, they propose the use of three different interconnected ontologies that contain general knowledge about discrete manufacturing processes, domain knowledge, and knowledge about ML-models. The creation of the domain ontology is done collaboratively by domain experts and data experts using a GUI developed in [7] called ontology extender. The idea here is similar to the approach we use to create an ontology that depicts the manufacturing process. However, the methodology in [6,7] is shown only for individual process steps and does not include the depiction of an entire manufacturing process. In addition, they do not provide a procedure for how to model a manufacturing process and its parameters.

The rest of this paper is organized as follows. In Section 2, we give a brief overview of ontologies and explain the one we have created and how we can use it to depict arbitrarily large manufacturing processes in a structured way. In Section 3, we depict the manufacturing process of calcium silicate bricks to provide a qualitative evaluation of our ontology. In Section 4, we present how we can use the ontology we created to answer the six questions we defined above. We also explain how we can use our ontology to help us find alternative target variables as well as suitable data sources to model/predict them with ML-models. At the end, we summarize our methodology and results and provide a brief outlook for future research.

2 ONTOLOGY

In this section we give a brief introduction to ontologies. Afterwards, we describe the ontology we created to depict a manufacturing process and how we can apply it to a specific use case. The general idea of using the binary relations between individuals to create an ontology of a manufacturing process stems from the creation of the domain ontology in [6, 7].

2.1 Foundations

The ontology is modelled using OWL [8], which is based on Description Logics [9] formalizing its semantics, and Web technologies, (URIs, RDF/XML serialization) to make knowledge bases shareable. An OWL ontology is a set of axioms that make statements about a domain of interest. Domain elements are represented as OWL entities. Particularly, these are OWL individuals representing specific objects, OWL classes representing sets of individuals, and OWL properties representing directed relationships between individuals (object properties). If an object property is relating two individuals with each other, its inverse object property relates the two individuals in the opposite direction.

With axioms being truth statements about entities, they can describe class relationships, e.g. stating that a class is a subclass of another class allowing for the creation of complex class hierarchies. Other types of axioms are assertional axioms, stating, for instance, that an individual is a member (instance) of a specific class, or property-based axioms stating, for instance, that a property is a subproperty of another property. Another example of property-based axioms is transitivity. To this end, if an individual A is related via a transitive property p with individual B, and B is related via the same p with C, then A is related via p directly with C. A more general concept of this is the subproperty-chain, where for properties p, q, and r, and individuals A, B and C, we can describe that if A is related to B via p, and B is related to C via q, then A is related to C via r. Note that property-chains are not limited to two properties.

2.2 General Concepts

The common elements that are present in the description of any manufacturing process are defined as classes. Meanwhile, the possible relationships between the different elements are defined as object properties. For a particular use case, we depict a manufacturing process using individuals that we relate by assigning them to the given classes and using the given object properties.

Two general ideas are incorporated throughout the ontology. First, we defined an inverse for each object property. This way, we only need to define the relationships of the individuals we create in one direction, while the reasoner automatically completes the other one. Second, we sometimes use subproperties to describe the relationship between individuals more precisely. The idea is that we can define a transitive superproperty allowing us to use the reasoner of the ontology to give us additional information about the relationship between the individuals, while keeping the path that connects two individuals traceable.

2.3 Process Definition

We begin the description of a respective manufacturing process by defining the underlying major process steps and ordering them by defining the direct predecessors of each step, if it exists. Then, for each process step, we define the respective subprocess steps, if they exist, relate them to their superprocess step, and order them by defining the direct predecessor at the subprocess level. This structure is similar to the one presented in [4].

To gain as much knowledge as possible from the ontology, we define the direct predecessor of a process step using the object property "hasSameLevelDirectPredecessor". This property has "hasSameLevelPredecessor" as a transitive superproperty. This way the reasoner automatically provides us with all previous process steps on the same hierarchical level, while allowing us to trace the order of the process step following the direct predecessors or successors.

Furthermore, the "hasSameLevelPredecessor" object property has the "hasPredecessor" superproperty. In addition to the transitivity, we additionally defined a subproperty-chain that argues that every predecessor of a process step is also a predecessor of all its subprocess steps. This way, we only have to define the direct predecessors that exist on the same hierarchical level, while getting all other relations by automated inferencing.

2.4 Device Definition

We continue by defining all devices that are used during the manufacturing process. We do this in the order given by the process steps defined in the previous subsection, to guarantee a structured procedure. For each process step, we define the machines or, more generally, the devices used by it, as well as the respective machine parts and sensors that we consider worth mentioning explicitly. The latter are related to their respective machines using the object properties "isPartOf" and "isSensorOf" respectively.

We then define the computing devices used throughout the manufacturing process and relate them to the respective devices they control or receive inputs from. We distinguish between general computing devices such as PLCs and central computing devices such as cloud servers.

2.5 Material Definition

In the third step, we define all the materials used throughout the manufacturing process. Again, we follow the process steps defined in Subsection 2.3. For each step, we observe the machines used during it and relate them to the materials they take, consume or produce using the respective object properties. We further classify the materials we define as raw materials, intermediate products, or final products. If a material cannot be assigned to a certain machine, but only to a process step, we use the corresponding superproperties "isInputOf" and "isOutputOf". We also use subproperty-chains to classify any material that is taken, consumed or produced by a machine used during a process step, as input or output of that process step.

In addition, we relate each of these products to the materials from which it is directly made using the "directlyMadeFrom" property. This property has the transitive superproperty "madeFrom". Thus, the reasoner provides us with all the materials used in previous steps to produce our current product, while still allowing us to trace the order in which the products have been processed.

2.6 Parameter Definition

For each process step, we observe the machines and materials used in it and define the parameters for each one of these individuals. Then, we define the additional parameters that are assigned to the respective process step itself. When we define a new parameter, we classify it as either a static or continuous parameter. We call a parameter static if it does not change during the entire manufacturing process and call it continuous if it does.

When it comes to static parameters related to materials, we manually assign the parameters only to the material where they occur earliest in the manufacturing process. The idea behind this is that when an intermediate product is made from previous products, the static parameters of those pervious products are also static parameters of the intermediate product they produce. This logic is automatically applied by the reasoner of the ontology, meaning that we can observe any static parameter of an intermediate or final product, while only having to assign the respective parameters to the materials where they first occur. This avoids repetition and leads to a better conciseness when assigning the parameters to the respective materials.

We then assign all parameters that are computed, displayed or, an input to a computing device to that device. This allows us to trace where we can potentially collect data about these parameters later in the development process.

2.7 Parameter Relationship Definition

To complete our ontology, we go through each parameter in the order given by the process steps and define their relationship to each other. If a parameter is directly depending on another parameter, we assign them to each other using the "isDirectlyDependingOn" object property. This property again follows the logic of having a more general transitive superproperty. This allows us to get all the other parameters a particular parameter depends on, while still being able to identify direct dependencies and follow the path of dependencies throughout the manufacturing process. The general idea here is similar to [5]. However, we provide a much more detailed depiction of the relationships between parameters.

If more is known about the dependency of parameters, we can use additional subproperties we defined. If a parameter is explicitly calculated from some other parameters, we can express this using the "isCalculatedWith" object property. Additionally, we can define direct monotone proportional or inversely proportional dependencies using the respective object properties. These properties in turn have superproperties that follow the logic of nested proportional or inversely proportional dependencies.

Specifically, this means that the property of proportional dependence is transitive. Additionally, if parameter A is proportionally depending on parameter B, which is inversely proportionally depending on parameter C, the reasoner automatically assigns parameter A to be inversely proportionally depending on parameter C. The same logic is applied if the dependencies are in reverse order.

After defining all known relationships between the parameters, the manufacturing process is defined, including the respective parameters and the relationships between all individuals. We did this by following a clear structure and defining only direct relationships. This makes it possible for non-experts to build an ontology depicting a manufacturing process. What exactly we intend to use this depiction for and what knowledge we get from the reasoner of the ontology is explained in Section 4.

3 APPLICATION

In this section, we illustrate some of the ideas we implemented in our ontology by using it to depict the manufacturing process of calcium silicate bricks as a proof of concept. A partial overview of this ontology can be seen in Fig. 2. The entire ontology we created can further be found on GitHub (https://github.com/AImotion-Bavaria/MPPO).

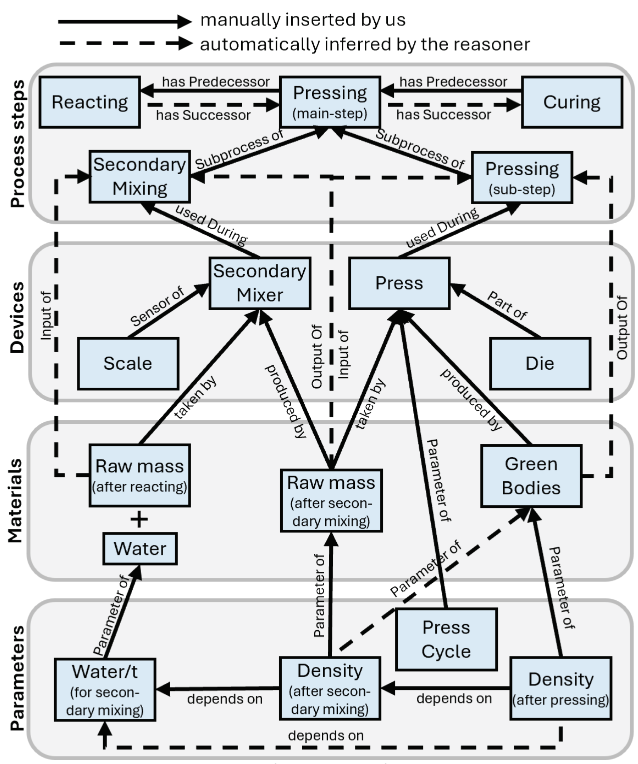

Figure 2 Partial depiction of the ontology for calcium silicate bricks

3.1 Manufacturing Process of Calcium Silicate Bricks

We begin this section with a brief summary of the calcium silicate bricks manufacturing process. It consists of five main process steps. First, the raw materials calcium oxide, sand, and water are mixed with additional aggregates to a raw mixture. This raw mixture is then required to react for approximately 30 to 120 minutes, before being pressed into green bodies of the respective format. Afterwards, the green bodies are cured in an autoclave in a steam atmosphere at a temperature of about 205 °C and pressure of about 14-16 bars. The curing process is by far the most energy-intensive processing step (approx. 80%) and at the same time the bottleneck in the production chain. At the end, the bricks are packaged for further transport. [10]

We start the ontology, by defining the five major process steps just mentioned, ordering them, and adding the respective subprocess steps.

3.2 Machines and Materials

After the process steps are defined, we add the devices and then the materials used in the manufacturing process, following the procedure described in Subsections 2.4 and 2.5.

We take a closer look at the materials we defined to explain the idea behind the "directlyMadeFrom" or "madeFrom" object property. Both the raw mixture and the final calcium silicate brick are made from the four raw materials mentioned in the previous subsection. However, we only manually add the first dependency to our ontology. But because we also meticulously track the transformation of the raw materials and intermediate products that lead to the final product throughout the manufacturing process, the reasoner automatically tells us that the raw mixture and the final calcium silicate bricks are made from the same four raw materials.

3.3 Parameters

As described in Subsection 2.6, we continue by adding the parameters to our ontology, assign them to their respective individuals, and define them as static or continuous, respectively. For static parameters of materials, we only assign them to the materials where they first occur. We elucidate the idea behind this by continuing the example from the previous subsection.

The raw materials have the parameter of their mixing ratio, i.e. how much of them is used to produce one ton of the raw mixture. Following the logic of a manufacturing process, the final product, i.e. the calcium silicate bricks, also have the parameter that describes the mixing ratio used to produce them. In order to avoid repetitive assignment of parameters, we included the idea explained in the second paragraph of Subsection 2.6. Since we included the transformation of raw and intermediate products in our ontology, the reasoner knows how the final product is made. In our case, this means that the reasoner automatically knows that the bricks are made from the initial raw mixture and automatically assigns them the respective static parameters such as their mixing ratio.

3.4 Parameter Relationships

In the final step, we define the relationships between the parameters, following the procedure described in Subsection 2.7. We want to use our example to illustrate the idea of the specific proportional and inversely proportional object properties.

Take, for example, the parameter of total emissions that are emitted during the curing process step. These are proportional to the amount of fossil fuel used which is proportional to the amount of fresh steam required for the curing the bricks. However, the amount of fresh steam required is inversely proportional to the amount of steam we reuse from previous curing processes [11]. While we only include these direct relations in our ontology, the reasoner automatically gives us any relationship between parameters that can be concluded from the logical rules we stated in Subsection 2.7. In this example, this means that the reasoner automatically tells us that the emissions emitted during the curing of the bricks are inversely proportional to the amount of steam we recycle from previous curing processes.

In general, the reasoner not only provides us with the parameters on which a certain parameter depends, but also with the direction of their relationship according to the logical rules mentioned above. This is especially useful for applications with even more parameters, where it is consequently easy to lose track of the exact dependencies between them.

4 UTILIZING THE ONTOLOGY

In this section, we describe what the ontology we created to depict a manufacturing process can be used for. Our initial goal was to create a methodology that can assist in bridging the gap between business and data understanding to apply ML-models that can help achieve predefined business goals.

4.1 Answering Questions about the Manufacturing Process

In the Introduction we defined six questions that may arise when trying to understand a manufacturing process with the idea of applying a ML-model to it. We present how we can answer these questions for a given manufacturing process using the ontology we created.

1) For each process step, we are provided with all subsequent and previous process steps and their respective hierarchy. The ontology also tells us the directly adjacent process steps, allowing us to follow the manufacturing process step by step. Further, we can see all devises utilized, as well as the materials used and produced during each process step.
2) For each device, we can observe what parts it is made of and which materials it uses and produces.
3) For each material, we can observe in which process step it is used, whether it is an input, output, or both to a particular machine/process step, what materials it is made from in previous process steps, and which subsequent materials are made from it in later process steps. For the latter two, we get additional information about which material it is directly made from or directly makes, allowing us to follow the manufacturing process in this way.
4) The ontology provides us with each parameter for each device, material, or process step and tells us whether the respective parameter is static or continuous. The ontology further allows us to distinguish between parameters that are directly related to materials and those that are inherited from input materials.
5) For each parameter, we can observe which parameters it depends on, and which parameters depend on it. We also get additional information about direct, proportional, and inversely proportional dependencies.
6) For each parameter, we can observe to which computing device it is connected, and whether it is displayed, computed, or an input to the respective device. Vice versa we also get all parameters that are received, displayed, or computed by a respective computing device.

4.2 Data Source and Target Variable Selection

As mentioned, determining the appropriate target variables and the respective relevant data sources is one of the key aspects when applying ML-models. For this reason, we take a brief look at queries and how we can use them to achieve these goals. We start by looking at how the ontology and queries can be used to determine suitable data sources.

Given a target variable, i.e. a parameter, we can simply define a short query that returns all the parameters on which the target variable depends. We can further specify this query. For example, we can state that we only want to see the parameters our target variable depends on that are actually connected to a computing device. As a result, we only get parameters that can potentially be acquired without having to install additional hardware. In general, we can use queries like the one described above to easily get a preselection of potentially relevant data sources for a ML-model. Then, additional methodologies such as [3] or interviews with domain experts can be used to further determine the exact data sources we want as our database.

In addition, we can use queries to help us determine alternative target variables if we are unable to acquire a suitable dataset for the current one. To do this, we define a query that returns all parameters in which our current target variable depends on proportionally or inversely proportionally. These are the potential candidates for alternative target variables, which have to be examined individually for their suitability as alternative target variables. The main criteria to consider is whether the alternative parameter captures all (or at least most) of the aspects of the original one, and whether we can acquire a suitable dataset for this parameter.

For a better understanding, consider the hypothetical business goal of reducing emissions. The majority of emissions are produced during the curing of the bricks [12]. Thus, the parameter "EmissionsAutoclaving" is an obvious choice for the target variable that we want to optimize. However, due to the layout of the machines, it is basically impossible to measure the emissions caused by a single autoclave or curing process [10]. But, using our ontology and a respective query, we can see that the emissions produced during the curing process are inversely proportional to the difference in pressure between the donating and receiving autoclaves, which can be calculated using the constantly recorded current pressure in the autoclaves making it an alternative target variable.

5 CONCLUSION

We developed a methodology for the detailed structural depiction of a manufacturing process using an ontology.

There, the reasoner, together with the logical rules that we created in the form of subproperty-chains, provides us with extensive knowledge about the relationships between the elements present in a manufacturing process. To this end, we only have to manually define binary relationships between the elements of our ontology. We also demonstrated how to use queries in our ontology to assist us determining practical target variables and selecting suitable data sources for them.

However, there are few limitations currently present in our methodology. The formalism of the ontology does not allow to define that if a parameter A is inversely proportionally dependent on a parameter B which is again inversely proportionally dependent on a parameter C, then parameter A is proportionally depending on parameter C. A possible workaround for this issue is to apply the reasoner in two steps and materialize the intermediate conclusions regarding the afore mentioned case of possible parameter relations, hence, breaking the cyclic dependencies. Such an implementation is a potential topic for future work.

Another possibility for future work involves the verification of the proposed methodology. We can test the capabilities of our ontology by using it to describe other manufacturing processes, or verifying the quality of the selected data sources or target variables by conducting empirical evaluations on the performance of ML models trained with the data sources and target variables suggested by our ontology.

Before doing such verification, some future work should be undertaken to extend our current ontology to avoid repetitiveness when depicting additional manufacturing processes. The general idea is to create modular ontologies which can be used to represent certain aspects that are present in multiple manufacturing processes, such as certain types of machines or even entire repetitive process steps. Such a modular decomposition of an ontology facilitates the reuse and sharing of partial knowledge formalized in several ontologies across different domains and use cases. Consequently, authoring and maintenance efforts to create additional ontologies can be drastically reduced.

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