

# Inferring SHACL Constraints for Results of Composable Graph Queries (Extended Abstract)

Philipp Seifer<sup>1</sup>, Daniel Hernández<sup>2</sup>, Ralf Lämmel<sup>1</sup> and Steffen Staab<sup>2,3</sup>

<sup>1</sup>University of Koblenz, Koblenz, Germany

<sup>2</sup>University of Stuttgart, Stuttgart, Germany

<sup>3</sup>University of Southampton, Southampton, UK

## Abstract

SPARQL CONSTRUCT queries allow for the specification of data processing pipelines that transform given input graphs into new output graphs. Input graphs are now commonly constrained through SHACL shapes allowing for both their validation and aiding users (as well as tools) in understanding their structure. However, it becomes challenging to understand what graph data can be expected at the end of a data processing pipeline without knowing the particular input data: Shape constraints on the input graph may affect the output graph, but may no longer apply literally, and new shapes may be imposed by the query itself.

In our recent work, *From Shapes to Shapes: Inferring SHACL Shapes for Results of SPARQL CONSTRUCT Queries*, we studied the derivation of shape constraints that hold on all possible output graphs of a given SPARQL CONSTRUCT query by axiomatizing the query and the shapes with the *ALCHOI* description logic. This extended abstract summarizes our previous work.

## Keywords

Semantic Queries, Data Pipelines, SHACL, SPARQL CONSTRUCT

## 1. Introduction


Some graph query languages are composable (i. e., they construct new graphs as results) and thereby allow for the fruitful composition of queries into data processing pipelines. Examples for such languages are SPARQL (in particular, its CONSTRUCT [1] queries) for RDF graphs and more recently G-CORE [2] for property graphs.


When graphs existing in the context of such composable query languages are validated using constraints specified in a shape description language such as SHACL [3] or ProGS [4], an interesting problem arises: Even though the input to a query is well-defined with SHACL or ProGS shapes, it becomes unclear which shapes apply after executing the query. Constraints that applied to the input graph may be invalidated by the query, e. g., because some required edges were removed, and new shapes may arise from the queries' construction template as well. Indeed, both downstream applications (e. g., programming languages [5]) and software developers working with graph data must understand what a query may output.


**Problem Description** In our recent paper [6], we define the problem of computing a set of SHACL shapes that characterises the possible output graphs of a SPARQL CONSTRUCT query. We represent queries as rules  $H \leftarrow P$  where the *template*  $H$  and *pattern*  $P$  are sets of assertions with variables. Bindings for variables in  $P$  are used to construct a new graph according to  $H$ . We express SHACL shapes as *ALCHOI* axioms (cf. [7]).

Formally, we define the problem **OUTPUTSHAPES** with signature  $(\mathcal{S}_{\text{in}}, q) \mapsto \mathcal{S}_{\text{out-max}}$ , where  $q$  is a query and  $\mathcal{S}_{\text{in}}$  and  $\mathcal{S}_{\text{out-max}}$  are two sets of shapes, called the *input* and *output* shapes. The set  $\mathcal{S}_{\text{out-max}}$

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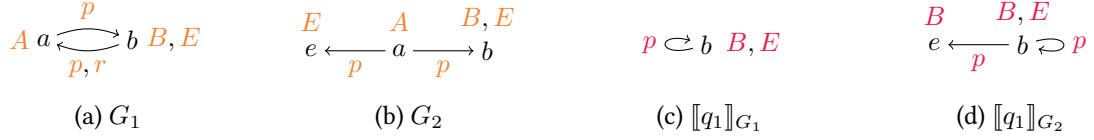
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 pseifer@uni-koblenz.de (P. Seifer); daniel.hernandez@ki.uni-stuttgart.de (D. Hernández); laemmel@uni-koblenz.de (R. Lämmel); steffen.staab@ki.uni-stuttgart.de (S. Staab)

 0000-0002-7421-2060 (P. Seifer); 0000-0002-7896-0875 (D. Hernández); 0000-0001-9946-4363 (R. Lämmel); 0000-0002-0780-4154 (S. Staab)



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**Figure 1:** (a,b) Input graphs for  $q_1$  valid with respect to  $S_1$ . (c,d) Results of  $q_1$  on  $G_1$  and  $G_2$ .

is the maximum set of shapes such that for every graph  $G_{\text{in}}$  that satisfies the input shapes – we write  $\text{valid}(G_{\text{in}}, \mathcal{S}_{\text{in}})$  – the graph resulting from evaluating  $q$  on  $G_{\text{in}}$ , denoted  $\llbracket q \rrbracket_{G_{\text{in}}}$ , satisfies the output shapes, i. e.,  $\text{valid}(\llbracket q \rrbracket_{G_{\text{in}}}, \mathcal{S}_{\text{out-max}})$ .

**Running Example** Consider a problem OUTPUTSHAPES with a query  $q_1$  and a set of shapes  $S_1$  as input. Let  $q_1 = \{y:E, z:B, (y, z):p\} \leftarrow \{(w, y):p, y:B, (x, z):p, z:E\}$ . Given a graph  $G_{\text{in}}$ , query  $q_1$  finds bindings for variable  $y$  that are  $B$ , and bindings for variable  $z$  that are  $E$ , both with incoming edges with role name  $p$  in  $G_{\text{in}}$ . Then, the query constructs the output graph,  $G_{\text{out}} = \llbracket q_1 \rrbracket_{G_{\text{in}}}$ , consisting only of these bindings for  $z$  and  $y$ , with inverted concept annotations and  $p$ -edges between them. Note, that we color-code the namespace of the input versus output graphs, since the extensions of the involved concept and role names are not the same.

Let  $S_1 = \{s_1, s_2, s_3\}$  where  $s_1 = A \sqsubseteq \exists p.B$ ,  $s_2 = \exists r.\top \sqsubseteq B$  and  $s_3 = B \sqsubseteq E$ . The graphs  $G_1$  (a) and  $G_2$  (b) in Figure 1 are valid with respect to  $S_1$ . Graphs  $\llbracket q_1 \rrbracket_{G_1}$  (c) and  $\llbracket q_1 \rrbracket_{G_2}$  (d) in Figure 1 are the respective output graphs for  $q_1$  over  $G_1$  and  $G_2$ , respectively.

Some expected output shapes are  $E \sqsubseteq \exists p.B$  and  $E \sqsubseteq B$ . The first shape follows directly from the query template. Each node labelled  $E$  has an outgoing edge to a node labelled  $B$ . The second shape  $E \sqsubseteq B$  is valid because  $B \sqsubseteq E$  holds on all input graphs: As a result, we can infer that all bindings for  $y$  are also bindings for  $z$ , such that  $E \sqsubseteq B$  follows from the query template.

**Proposed Algorithm** In this paper, we summarize the algorithm we presented in [6] (an extended version with proofs is available in [8]), which constructs a *sound* (but not *complete*) approximation  $\mathcal{S}_{\text{out}} \subseteq \mathcal{S}_{\text{out-max}}$ .

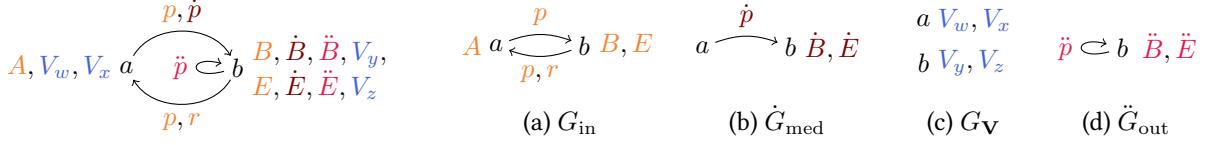
To this end, we split the problem into two subproblems: First, the problem of deciding whether any given shape must be included in the output, and secondly the problem of generating a set of candidate shapes. The second problem turns out to be rather trivial, as the set of candidates is finite: We consider a subset of SHACL that is (syntactically) finite for a finite vocabulary, and show that all relevant candidates are indeed from the finite vocabulary of the query. In our extended version, we show that this also holds for a much larger subset of SHACL.

Thus, we focus on the first problem in Section 2 and Section 3.

## 2. Axiomatizations Over Query Executions

As hinted earlier, different occurrences of the same concept name do not have the same extensions: A query matches on input graphs, determines valuations (as subsets of the input), and constructs new graphs. We distinguish between the inputs, intermediate bindings, as well as the constructed output by rewriting input symbols  $A, p$  into *fresh* symbols  $\dot{A}, \dot{p}$  after the first step, and into  $\ddot{A}, \ddot{p}$  after the second step. These rewritten symbols allow us to encode assertions that are valid for only specific states of query execution. Variable bindings, on the other hand, hold throughout: We codify a variable binding  $\mu(x) = a$  as a concept assertion  $a:V_x$ , where  $V_x$  is a fresh concept name.

In order to axiomatize how (all possible) input graphs are connected to (all possible) output graphs, we define a (virtual) *extended graph*  $G_{\text{ext}}$ , that unifies the different steps, and therefore allows us to reason about them:  $G_{\text{ext}} := G_{\text{in}} \cup \dot{G}_{\text{med}} \cup G_{\mathbf{V}} \cup \ddot{G}_{\text{out}}$ , where  $G_{\text{med}}$  is  $\bigcup_{\mu(P) \subseteq G_{\text{in}}} \mu(P)$  (i.e., the union of all graphs  $\mu(P)$  resulting from replacing every variable  $x$  in  $P$  with  $\mu(x)$ ),  $\dot{G}_{\text{out}}$  is  $\llbracket q \rrbracket_{G_{\text{in}}}$ , and  $G_{\mathbf{V}}$  is the graph containing an assertion  $a:V_x$  if and only if there exists a valuation  $\mu$  such that  $\mu(P) \subseteq G_{\text{in}}$



**Figure 2:** On the left the graph  $G_{\text{ext}}$  as the union of  $G_{\text{in}}$  (a),  $\dot{G}_{\text{med}}$  (b),  $G_{\text{V}}$  (c), and  $\ddot{G}_{\text{out}}$  (d).

and  $\mu(x) = a$ . Figure 2 shows the extended graph and its components for the running example query  $q_1$ , and the graph  $G_1$  in Figure 1 .

**Proposition 1.** *Given a graph  $G_{\text{in}}$  and a query  $q$ , let the graphs  $G_{\text{ext}}$ ,  $G_{\text{med}}$ , and  $G_{\text{out}}$  be the extended graph and its components. For every axiom  $\varphi$  that does not include names with dots (e. g., names  $\dot{A}$ ,  $\ddot{A}$ ,  $\dot{p}$ , or  $\ddot{p}$ ), the following equivalences hold:  $\text{valid}(G_{\text{in}}, \{\varphi\})$  if and only if  $\text{valid}(G_{\text{ext}}, \{\varphi\})$ ,  $\text{valid}(G_{\text{med}}, \{\varphi\})$  if and only if  $\text{valid}(G_{\text{ext}}, \{\dot{\varphi}\})$ , and  $\text{valid}(G_{\text{out}}, \{\varphi\})$  if and only if  $\text{valid}(G_{\text{ext}}, \{\ddot{\varphi}\})$ .*

Given the notion of extended graphs, we can prove Proposition 1 (see [8] for the proof), which is essential to our method. Utilizing this proposition, we can show as a corollary that given a set of axioms  $\Sigma$  such that  $\text{valid}(G_{\text{ext}}, \Sigma)$  for all extended graphs of a query  $q$ , if  $\Sigma \models \ddot{s}$  then  $\text{valid}(G_{\text{out}}, \{s\})$  for every output graph  $G_{\text{out}}$  of  $q$ . Thus, what remains is to show how to construct such a set of axioms  $\Sigma$ .

### 3. Axioms Valid on Extended Graphs

Let us now consider what axioms can be inferred, by inspecting the running example. First, we can notice that the input shapes  $\mathcal{S}_{\text{in}}$  are valid on all input graphs, by definition. Thus, we include them in our knowledge base  $\Sigma$ .

Some axioms of the validation knowledge base (unique name, closed world and domain closure assumptions) can be approximated by investigating the query  $q$ . The unique name assumption is limited to individual names that occur in the query; in the running example there are none. Since a query does not determine the set of individual names, no axioms related to the domain closure assumption can be inferred. On the other hand, a query does restrict concept names that appear in the query with respect to the closed world assumption (CWA).

For the running example, we can thus infer  $\{\dot{B} \equiv B \sqcap V_y, \dot{E} \equiv E \sqcap V_z\}$ , because e. g., concept  $\dot{B}$  in the extended graph is defined by filtering  $B$  with variable  $V_y$ , based on the query pattern  $y:B$  in  $q_1$ . We can also infer axioms  $\{V_w \equiv \exists p.V_y, V_x \equiv \exists p.V_z, V_y \equiv \exists p.V_w \sqcap B, V_z \equiv \exists p.V_x \sqcap E\}$  since variable concepts are defined by constraints to the variable in the query pattern. For example,  $V_y$  is constrained by patterns  $(w, y):p$  and  $y:B$  in  $q_1$ , and thus bound by  $\exists p.V_w \sqcap B$ . This is a crucial step, since concept and role names in the extended graph are defined in terms of these variable concepts:  $\{\ddot{B} \equiv V_z, \ddot{E} \equiv V_y\}$  since e. g., concept  $\ddot{B}$  in the extended graph is defined by  $V_z$ , as it only occurs in the single construct pattern  $z:B$ . With similar reasoning,  $\{\exists \dot{p}.V_y \equiv V_w, \exists \dot{p}.V_z \equiv V_x, \exists \dot{p}.\top \equiv (V_w \sqcap \exists \dot{p}.V_y) \sqcup (V_x \sqcap \exists \dot{p}.V_z)\}$  as well as  $\{\exists \ddot{p}.V_z \equiv V_y, \exists \ddot{p}.\top \equiv V_y \sqcap \exists \ddot{p}.V_z\}$  (and their inverse counterparts) can be constructed with respect to role names.

Query  $q_1$  has two components  $P_1 = \{(w, y):p, y:B\}$  and  $P_2 = \{(x, z):p, z:E\}$  not sharing variables. The CWA encoding does not entail  $V_y \sqsubseteq V_z$ , even though this axiom is both valid in all extended graphs, and required for inferring, e. g., the result shape  $E \sqsubseteq B$ . In another step of the algorithm, we infer these additional subsumptions by constructing variable mappings  $h$  between query components, that are potentially extended with input shapes. In this case, we know based on input shape  $S_1$  that  $B \sqsubseteq E$ . We can utilize this knowledge to extend component  $(w, y):p, y:B$ , adding the pattern  $y:E$  which does not alter the queries results. Then, we can find the mapping  $h(x) = w, h(z) = y$  such that  $h(P_2) \subseteq P_1$ , which implies  $V_w \sqsubseteq V_x$  and  $V_y \sqsubseteq V_z$ .

## 4. Conclusion

We presented an algorithm for inferring a set of shapes that validate the possible output graphs of a CONSTRUCT query, where input graphs of this query can be constrained by a set of shapes as well. This enables the inference of shapes over result graphs of data processing pipelines (i. e., compositions of CONSTRUCT queries), which can be used both for validation purposes when working with these result graphs, and informatively, aiding developers directly.

Our approach differs from related work (e.g., [9, 10, 11, 12, 13, 14]) in that we infer shapes from statically known information (query and input shapes) and not from instance data. Thus, it is similar to approaches for inferring constraints over views on relational databases (e.g., [15, 16, 17, 18]), but utilizing a modelling approach that is feasible and supports crucial constraints for typing knowledge graphs. Some approaches construct SHACL from static information [19, 20, 21], such as RML rules or direct mappings, though they are limited in either a less expressive mapping language, or lack support for constraints on the input data. An implementation [22] for the algorithms presented in our work is available on GitHub<sup>1</sup>.

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