Validation and Inference of Schema-Level Workflow Data-Dependency Annotations

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Abstract. An advantage of scientific workflow systems is their ability to collect runtime provenance information as an execution trace. Traces include the computation steps invoked as part of the workflow run along with the corresponding data consumed and produced by each workflow step. The information captured by a trace is used to infer "lineage" relationships among data items, which can help answer provenance queries to find workflow inputs that were involved in producing specific workflow outputs. Determining lineage relationships, however, requires an understanding of the dependency patterns that exist between each workflow step's inputs and outputs, and this information is often under-specified or generally assumed by workflow systems. For instance, most approaches assume all outputs depend on all inputs, which can lead to lineage "false positives". In prior work, we defined annotations for specifying detailed dependency relationships between inputs and outputs of computation steps. These annotations are used to define corresponding rules for inferring fine-grained data dependencies from a trace. In this paper, we extend our previous work by considering the impact of dependency annotations on workflow specifications. In particular, we provide a reasoning framework to ensure the set of dependency annotations on a workflow specification is consistent. The framework can also infer a complete set of annotations given a partially annotated workflow. Finally, we describe an implementation of the reasoning framework using answer-set programming.

1 Introduction

Within most scientific workflow systems, a *workflow specification* (or *schema*) is modeled as a graph of nodes representing computational steps and edges representing the data and control flow between steps [5,10]. Each workflow step in a specification is typically treated as a "black box" by the workflow system. For example, steps are frequently configured to invoke external programs, execute scripts, or call web services, where the step exposes only the inputs needed and the corresponding outputs returned by the underlying calls. Once designed, workflow specifications serve as executable and potentially reusable (e.g., using different input data and parameter settings) scientific analyses. Because scientific workflow systems invoke and control the flow of data between steps during workflow execution, most systems provide support for recording (or logging) information about a workflow run. A *workflow trace* stores information associated with a run as an instance of a workflow specification [5,2]. In particular, traces are modeled as graphs with nodes representing the invocations of steps and edges representing the data passed between each step's execution. Traces are often used to infer the lineage of workflow data products. For instance, given a data product output by a run, many systems use the trace to determine the steps that were invoked as well as the input and intermediate data products that contributed to its generation [5,2].

However, because steps in a workflow specification are black boxes, workflow systems often "overestimate" the lineage relationships from a workflow trace [2]. For instance, many systems assume that all data input to a step is used to produce all outputs, when in fact only a portion of input data may produce any particular output [4,2]. Additionally, most systems consider only a single, often underspecified notion of dependency between a step's inputs and outputs, e.g., where data items are said to be "influenced by" or "contribute to" other data items [3]. Taken together, the lineage information inferred from workflow traces may result in lineage relationships that are not only unclear, but often misleading or even incorrect.

In prior work [2], we developed a set of declarative rules for specifying dependency patterns of individual computation steps. The inputs and outputs of a step are annotated with rules, which are then used to infer the specific input data used to produce an output for each invocation of a step within a trace. However, to be effective, this approach requires a complete set of annotations for every step within a workflow specification.

Contributions. We describe extensions to our prior work that supports partially annotated workflow specifications and employs reasoning techniques to validate and help infer a complete set of annotations. We consider different use cases related to annotating a workflow specification and provide a set of dependency types that can be used to help clarify the lineage relationships present within a workflow trace. Finally, we describe a prototype implementation of our approach (implemented using answer-set programming) that we plan to add to the YesWorkflow system [11] as future work.

Organization. In Section 2 we describe an abstract model of workflow specifications, give an overview of the dependency types we consider for annotations, and discuss use cases related to our framework. In Section 3 we describe the constraints associated with the dependency types as well as the corresponding inferences for reasoning over partially annotated workflow specifications. In Section 4 we present a prototype implementation of the reasoning approaches described in Section 3. Finally, in Sections 5 and 6 we describe related and future work, respectively.

2 Workflow Dependency Annotations

This section describes an abstract model for workflow specifications used in the rest of the paper, an overview of the types of dependencies we consider for workflow annotations, and three example use cases related to annotation inference.

Workflow Specifications. We consider an abstract workflow model that conforms to YesWorkflow [11] and similar dataflow-oriented scientific workflow models [5,2]. A workflow $W = (P, D, E)$ consists of a set of *program blocks* P (workflow steps, i.e., computations), *data blocks* D (representing data items or data containers), and *input* and *output* edges $E \subseteq P \times L \times D \times \{\mathtt{in}, \mathtt{out}\}$ where L is a set of labels that uniquely identify

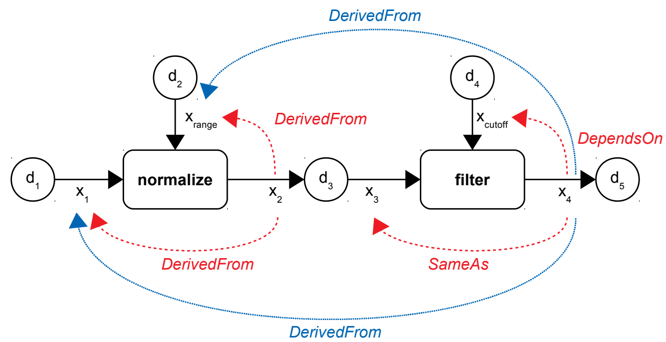


Fig. 1. Example workflow with program blocks `normalize` and `filter`, data blocks $d_1, \ldots, d_5$, and dataflow edges (solid, black) between nodes; user-declared dependency annotations (dashed, red edges); and inferred dependencies (dotted, blue edges), based on the given user annotations.

edges within W. We use relations $\texttt{in}(p_i, x_i, d_i)$ and $\texttt{out}(p_j, x_j, d_j)$ to denote input and output edges, respectively, for $p_i, p_j \in P$, $x_i, x_j \in L$, and $d_i, d_j \in D$. Figure 1 shows an example workflow consisting of two program blocks (`normalize` and `filter`), five data blocks ($d_1, \ldots, d_5$), four input edges (x_1, x_3, $x_{\texttt{range}}$, and $x_{\texttt{cutoff}}$), and two output edges (x_2 and x_4). Also shown in Figure 1 are a set of initial dependency annotations (red, dashed) together with the corresponding inferred annotations (blue, dotted). The `normalize` block takes input data items d_1 and scales them to fit within the given range (consisting of a minimum and a maximum value). The output of `normalize` is then passed to `filter`, which outputs the data item if it is smaller than a given cutoff value d_4. In general, an input edge $\texttt{in}(p_1, x_1, d_1)$ states that data items are input to the program block p_1 and an output edge $\texttt{out}(p_1, x_2, d_2)$ states that data items are output by p_1. Data blocks allow for data items to be passed as input to multiple program blocks (e.g., to create workflow branches as in d_2 in Figure 4). In contrast, data blocks typically receive only from a single writer, to avoid conflicts (e.g., $d_3 \neq d_4$ in Figure 4).[3]

Dependency Annotations. The set of dependency annotations $A \subseteq L \times L \times T$ for a workflow specification W associates different dependency types $t \in T$ to input and output edges of W. Dependency annotations are represented by a relation $\texttt{dep\_rule}(x_1, x_2, t)$ for input edges $x_1 \in L$, output edges $x_2 \in L$, and dependency types $t \in T$. The dashed, red arrows in Figure 1 represent four explicit, user-supplied annotations: $\texttt{dep\_rule}(x_1, x_2, \texttt{DerivedFrom})$, $\texttt{dep\_rule}(x_{\texttt{range}}, x_2, \texttt{DerivedFrom})$, $\texttt{dep\_rule}(x_3, x_4, \texttt{SameAs})$, and $\texttt{dep\_rule}(x_{\texttt{cutoff}}, x_4, \texttt{DependsOn})$. In the example, we say that the output of `normalize` is "*derived from*" the input d_1 and the `range` d_2, and the output of `filter` "*depends on*" the `cutoff` d_4 and is the "*same (data item) as*" the input d_2. We note that annotations can be expressed over a single program block (e.g., the explicit annotations in Figure 1) or can span multiple program blocks (e.g., the inferred annotations in Figure 1).

Dependency Types. We consider a set of pairwise disjoint dependency types for specifying annotations. The *FlowsFrom* type simply represents the cases where an input data item was received and an output item was produced by a program-block invocation, but the output value is not determined by or computed from the input. A *FlowsFrom* anno-

[3] If data blocks denote containers (e.g., file folders or queues) multiple writers may be allowable.

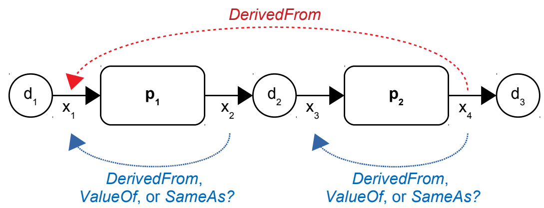


Fig. 2. Example workflow with initial user annotation (dashed, red) from the output x_4 to the input x_1. Which of the undeclared dependency options (dotted, blue) are correct?

tation typically denotes that the input is simply a "trigger" to tell the program block to be invoked. The *DependsOn* type represents cases where a control dependence exists between the corresponding inputs and outputs (explained in more detail in Section 3). The *DerivedFrom* type represents cases where outputs are computed from inputs (again, described further in Section 3). The *ValueOf* type represents the cases where an output produces a new data item (with a new object identifier) containing a copy of the input data item's value. Finally, the *SameAs* type represents the cases where the input data item was passed through to the output (i.e., the output is the same exact data item as the input data item).

Use Case 1: Inferring Dependency Annotations. Given a workflow specification that is partially annotated, we consider the case of inferring new annotations from a given set of user-supplied annotations. Figure 1 gives a simple example where each program block is annotated (dashed, red arrows) and the corresponding annotations that are implied by the given annotations are also shown (blue arrows). In this example, each individual workflow step is annotated by a user, and the goal is to infer the annotations that span multiple steps. In general, understanding the dependency relationships that span workflow steps as a result of the composition of program blocks is useful for verifying the intent and/or construction of the workflow (e.g., to ensure that certain workflow outputs are actually derived from certain workflow inputs). Having a complete set of annotations is also useful when answering queries at the trace level, e.g., to determine the inputs that specific outputs were derived from (as opposed to the inputs that were simply copied from the input or were used for basic control flow).

Use Case 2: Constraining Dependency Annotations. In this case, higher-level annotations that span multiple program blocks (e.g., between workflow inputs and outputs) are used to help guide annotation choices for the rest of the workflow specification. As a simple example, we may know that the output is (or should be) derived from the input as shown in Figure 2 by the dashed red annotation. Specifying this annotation first limits the choices for the lower-level annotations (in this case of program blocks). The corresponding choices are shown by the dotted blue annotations in Figure 2. In this case, different combinations of annotations over the two program blocks are compatible (consistent) with the initial (dashed red) annotation of Figure 2.

Use Case 3: Validating Dependency Relationships. Finally, we consider the case where there is a mix of (potentially partial) higher-level (i.e., indirect) and lower-level (i.e., direct) annotations of a workflow specification that a workflow designer wants to ensure are compatible (consistent). Figure 3 is one such example where the workflow specification consists of a subworkflow (named `generate_sample` as shown on

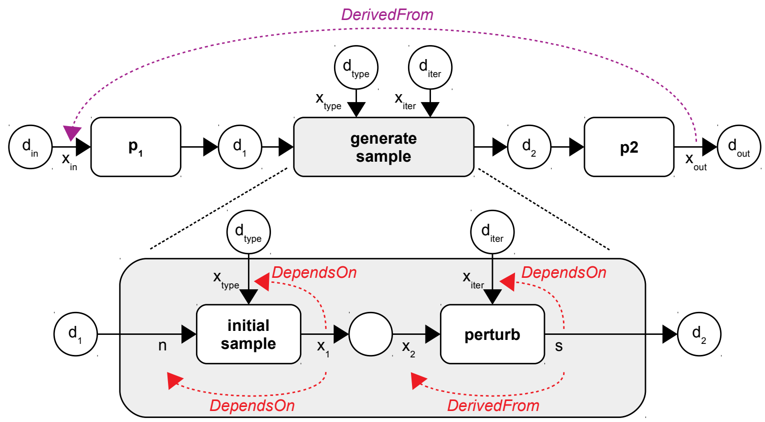


Fig. 3. Workflow specification consisting of an annotated subworkflow (dashed red, bottom) and an inconsistent higher-level annotation assertion (dashed purple, top) that spans workflow steps.

the bottom of the figure). Each subworkflow step is annotated (in red) and the containing workflow (shown on the top of the figure) has a higher-level annotation asserting that the output should be derived from the input. However, the given annotations are incompatible (i.e., inconsistent) since the composition of the two subworkflow steps introduce an implied *DependsOn* relationship between the input and output of `generate sample`. Thus, based on the workflow specification, $d_{\mathtt{in}}$ and $d_{\mathtt{out}}$ cannot participate in a *DerivedFrom* relationship (as shown at the top in purple).

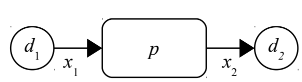
The reasoning framework we describe in the rest of this paper is designed to handle each of these three cases. In particular, we assume that a workflow specification is either fully or partially annotated, from which the reasoning framework (i) ensures consistency of the given annotations (e.g., as in Figure 3); (ii) infers all specific implied annotations (e.g., as in Figure 1); and (iii) provides the allowable annotation options when there are multiple possible implied annotations (e.g., as in Figure 2).

3 Reasoning over Dependency Types

This section describes our reasoning framework for dependency type validation and inference. We first give a more detailed description of the annotation types and then describe the annotation composition rules and constraints used within our framework.

3.1 Dependency Types

In the following, we assume a simple program block p with input edge $\mathtt{in}(p,x_1,d_1)$ and output edge $\mathtt{out}(p,x_2,d_2)$ as shown below.



Let D_1 be the set of allowable values (the *domain*) of p with respect to the input edge x_1 and D_2 be the set of possible output values (the *range*) with respect to the output edge x_2. We write $p : D_1 \to D_2$ to denote the *signature* of p with respect to x_1 and x_2. We assume data items are passed to and from program blocks as objects o with unique identifiers $id(o)$ and corresponding values $val(o)$. For a domain D and a sequence of data items $\bar{o}$, we write $val(\bar{o}) \subseteq D$ if for every data item $o_i \in \bar{o}$, $val(o_i) \in D$. Given the program block signature $p : D_1 \to D_2$, an *invocation* $p(\bar{o}_1) = \bar{o}_2$ states that p read a sequence of data items $\bar{o}_1$ on x_1 such that $val(\bar{o}_1) \subseteq D_1$, and wrote a (possibly empty) sequence of data items $\bar{o}_2$ on x_2 such that $val(\bar{o}_2) \subseteq D_2$.[4] Program blocks are not required to be deterministic, and so different invocations over the same input may produce different output. The *image* $p[\bar{o}_1]$ of $\bar{o}_1$ under p is the set of all possible output sequences produced by invocations of p receiving $\bar{o}_1$. Note that if p has multiple input edges, the same notion of image still applies since we are interested in the relationship between a single input and output edge (although additional constraints are imposed in some cases as described below).

Following the traditional convention used in programming language implementation [7,3], we use the ideas of "control" and "data" dependence between statements when defining the dependency types below. For example, consider the following statements (adapted from [7]).

```
S1: C = A * B
S2: E = C * D + 1
S3: if (E > 0) then
S4:    H = F + G
```

Statement `S2` is said to have a *data dependence* on `S1` since the value of `E` depends on the value of `C`. A data dependence is also referred to as a "*read-after-write*" dependence since `C` is read as part of `S2` to compute a value to write to `E`. Note that data dependence relationships can either be direct or indirect. For instance, in the example above, `E` directly depends on `C` (via `S2`) but indirectly depends on `A` (via `S1` and `S2`). Below, we write $\texttt{raw\_dep}(p, x_1, x_2)$ to denote that within a program block p, output edge x_2 has either a direct or indirect read-after-write dependence on input edge x_1. Similarly, statement `S4` is said to have a *control dependence* on statement `S3` since the execution of statement `S4` (and hence, the value of `H`) depends on the execution of `S3` (specifically, the value of `E`). However, note that `H`'s value is not computed from `E`'s value (which would imply a data dependence). A control dependence can also be either direct or indirect. We assume that if an x_2 is indirectly control dependent on x_1 then either: (i) x_2 is control dependent on another variable that is either directly or indirectly control or data dependent on x_1; or (ii) x_2 is data dependent on a variable that is either directly or indirectly control dependent on x_1. Below, we write $\texttt{ctl\_dep}(p, x_1, x_2)$ to denote that x_2 has either a direct or indirect control dependence on x_1. We define the dependency types below in terms of the constraints they impose between possible inputs and outputs of program-block invocations as well as their corresponding control and data dependences.

FlowsFrom. A *FlowsFrom* annotation implies that x_2 does not have a control or data dependence on x_1, which is expressed by the constraint:

$$\neg\,\texttt{ctl\_dep}(p, x_1, x_2) \;\wedge\; \neg\,\texttt{raw\_dep}(p, x_1, x_2).$$

[4] The use of sequences of data items allows for more complex program blocks such as filters and aggregators as well as workflow computation models supporting implicit iteration [1,2].

FlowsFrom simply suggests that the input was present when p was executed, e.g., the input was used as a "trigger" to invoke a program block p.

DependsOn. A *DependsOn* annotation implies that x_2 has a control dependence, but not a data dependence on x_1, which is expressed by the constraint:

$$\texttt{ctl\_dep}(p,x_1,x_2) \wedge \neg\, \texttt{raw\_dep}(p,x_1,x_2).$$

DerivedFrom. A *DerivedFrom* annotation implies that x_2 has a data dependence on x_1, but that not all outputs have the same value(s) as their corresponding inputs (which would suggest a *ValueOf* or *SameAs* relationship):

$$\texttt{raw\_dep}(p,x_1,x_2) \wedge (\exists \bar{o}_2 \in p[\bar{o}_1] : val(\bar{o}_2) \not\subseteq val(\bar{o}_1)).$$

As explained further below, we consider *DerivedFrom* to be a "stronger" dependency relationship than *DependsOn*. Thus, while it is possible for x_2 to have both a control and data dependence on x_1, it would be represented as *DerivedFrom* within our framework.

ValueOf. A *ValueOf* annotation implies that the values of data items received on x_1 are output on x_2 (e.g., by copying inputs to new outputs). Unlike with *SameAs*, *ValueOf* assumes new data items are created as a result, and so the identifiers for the input and output data items differ:

$$(\forall \bar{o}_2 \in p[\bar{o}_1] : val(\bar{o}_2) \subseteq val(\bar{o}_1)) \wedge (\exists \bar{o}_2 \in p[\bar{o}_1] : id(\bar{o}_2) \not\subseteq id(\bar{o}_1)).$$

We use $id(\bar{o})$ to denote the set of identifiers of the sequence of data items $\bar{o}$. Note that *ValueOf* implies a data dependence from x_2 to x_1 since data items must be read from input x_1 and then written into data items that are output to x_2.

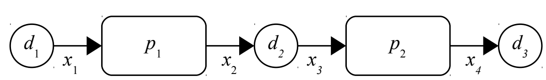
SameAs. A *SameAs* annotation differs from *ValueOf* by requiring all outputs to be the same as data items from the inputs:

$$\forall \bar{o}_2 \in p[\bar{o}_1] : o \in \bar{o}_2 \to o \in \bar{o}_1.$$

Here, $o \in \bar{o}$ holds if the object o is a member of the sequence $\bar{o}$. A *SameAs* relationship also implies a data dependence from x_2 to x_1 since the input data items must be read from x_1 and then written to x_2.

3.2 Composing Dependency Annotations

Annotation inference within a workflow specification is largely based on understanding how annotations "propagate" under compositions (or "sequences") of workflow steps. Here we assume two connected program blocks $p_1 : D_1 \to D_2$ and $p_2 : D_2 \to D_3$:



When p_1 and p_2 are connected by a data block as above, we write $p_1 \circ p_2$ to denote the connection. We also define the ordering $\prec$ to represent the intuitive "dependency strength" of annotation types. In particular, if $t_i \prec t_j$ then we say t_i is a "weaker" dependency type than t_j (or similarly, that t_j is a "stronger" dependency type than t_i). The dependency types are ordered according to dependency strength as follows.

$$FlowsFrom \prec DependsOn \prec DerivedFrom \prec ValueOf \prec SameAs$$

For instance, a *DependsOn* relationship suggests a "weaker" dependency than a *DerivedFrom* relationship. The definitions of the annotation types with the ordering above imply the following annotation composition rules for a sequence of program blocks $p_1 \circ p_2$, with $\mathtt{in}(p_1,x_1,d_1)$, $\mathtt{out}(p_1,x_2,d_2)$, $\mathtt{in}(p_2,x_3,d_2)$, and $\mathtt{out}(p_2,x_4,d_3)$ as defined above, and $\preceq$ denoting weaker or of equal strength (and where all variables are assumed below to be universally quantified).

$$\mathtt{dep\_rule}(x_1,x_2,t_i) \wedge \mathtt{dep\_rule}(x_3,x_4,t_j) \wedge t_i \preceq t_j \leftrightarrow \mathtt{dep\_rule}(x_1,x_4,t_i)$$
$$\mathtt{dep\_rule}(x_1,x_2,t_j) \wedge \mathtt{dep\_rule}(x_3,x_4,t_i) \wedge t_i \preceq t_j \leftrightarrow \mathtt{dep\_rule}(x_1,x_4,t_i)$$

These rules can also be applied to indirect annotations (spanning multiple blocks) as well, which is further described in Section 4. As an example of propagation, in Figure 1, `normalize` has a *DerivedFrom* annotation and `filter` has a *SameAs* annotation. Since *DerivedFrom* is "weaker" than *SameAs*, the composite annotation is *DerivedFrom*. Similarly, in Figure 2 the composite annotation is *DerivedFrom*, which implies that p_1 and p_2 have either *DerivedFrom* annotations or "stronger" types (i.e., *ValueOf* or *SameAs*), since *DerivedFrom* must be the "weaker" annotation. Additionally (and not shown in Figure 2), note that at least one of p_1 or p_2 must have a *DerivedFrom* annotation to satisfy the composition rules above. The example in Figure 3, while slightly more complex, follows the same idea in that along the path from $\mathtt{x_{out}}$ to $\mathtt{x_{in}}$, the `generate_sample` subworkflow implies a *DependsOn* annotation, and since *DependsOn* is strictly weaker than *DerivedFrom*, the higher-level *DerivedFrom* annotation violates (is inconsistent with) the composition rules.

According to the composition rules, weaker annotations propagate through program-block compositions, which is due to the nature of the dependencies established by the weaker annotation. For instance, if x_2 *FlowsFrom* x_1, then d_2 (via x_2) does not have a control or data dependence on d_1 (via x_1). Thus, since the value of d_1 does not participate in the computation of d_2, d_1 also does not participate in the computation of the values that have a control or data dependence on d_2. A similar situation exists when p_2 has a *FlowsFrom* annotation. Determining indirect control dependences (i.e., when looking at sequences of statements involved in control and data dependences) was described in the beginning of this section, and follows from the idea that control dependence can be indirectly established through other control and/or data dependences. The same ideas apply to copying the values of data items. If d_2 is a (value) copy of d_1 with potentially different data item identifiers as d_1 (i.e., x_2 has a *ValueOf* relationship with x_1), but d_2 is passed through to d_3 (i.e., x_4 has a *SameAs* relationship with x_3), then d_3 will also have the same value but a different identifier as d_1 (since d_2 and d_3 are the same data item). The same situation occurs when the two annotations are flipped, i.e., p_1 has a *SameAs* relationship and p_2 has a *ValueOf* relationship. Finally, when p_1 and p_2 have the same exact annotation, the same annotation is also propagated, which follows from similar arguments as those above.

3.3 Additional Annotation Constraints

We also consider an additional "global" constraint on the dependency annotations of a workflow specification related to inferring annotations when there are two or more paths

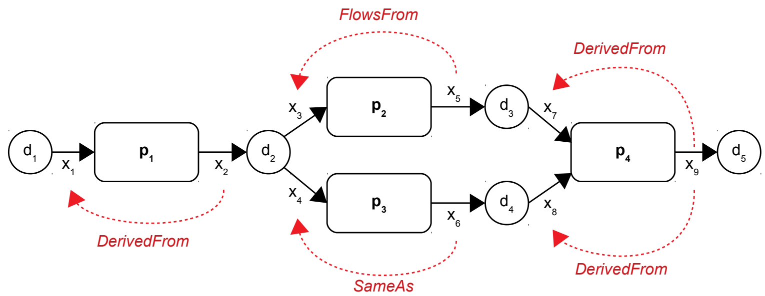


Fig. 4. Example workflow specification with multiple paths between the input and output.

of program-block compositions within a workflow specification. Consider the example annotated workflow specification of Figure 4, which shows two paths (i.e., sequences of program block compositions) between x_1 and x_9. While the top path (through p_2) implies a *FlowsFrom* relationship from x_9 to x_1 (since *FlowsFrom* is the weakest type along the path), the bottom path implies a stronger *DerivedFrom* relationship from x_9 to x_1. Since we allow at most one dependency type between an input and an output, we use the annotation inferred from the path with the strongest type.

4 Prototype Implementation

This section describes a prototype implementation of our annotation reasoning framework using the Potassco[5] suite of answer-set programming (ASP) tools. Potassco implements ASP using a syntax similar to Datalog with additional support for nonmonotonic reasoning based on the answer set semantics [8]. Potassco programs are often written using a generate-and-test algorithmic approach where the result of a program is a set of minimal models, or "*answer sets*", that satisfy the rules and constraints defined within the program. Our implementation follows this same approach by:

(i) "guessing" dependency annotations for each input-output pair in a workflow specification without a corresponding user-supplied annotation (the generate step);

(ii) ensuring that each of the input-output pair annotations satisfy the program-block annotation compositions described in the previous section (the test step); and

(iii) ensuring that annotations satisfy the additional constraints described in the previous section, i.e., ensuring the "strongest" indirect annotations are used between inputs and outputs with multiple paths of program blocks between them (the test step).

In the generate-and-test approach, conceptually all possible models are created—which in our case means that all possible combinations of input-output pair combinations along a dataflow path are considered—and only those models (answer sets) that satisfy the given constraints are returned. Our prototype implementation uses the answer sets for a workflow specification and then (i) outputs all annotations that are contained in each answer set (i.e., the annotations that are "entailed" by the program); and then (ii) outputs the annotation choices (i.e., the union of annotations across answer sets) for

[5] See: https://potassco.org/

the annotations that are not entailed (e.g., as is the case with the blue annotations in Figure 2).

Our prototype uses a "choice rule" to generate annotations for input-output pairs not already annotated as part of the workflow specification:

```
{dep_rule(I,O,R) : dep_type(R)} = 1 :- up_stream(I,O).
```

Where `up_stream(I,O)` finds all potential input-output annotation pairs:

```
up_stream(I,O) :- in(I,P,_), out(O,P,_).
up_stream(I,O) :- in(I,P1,_), out(O1,P1,D1), in(I2,P2,D1), up_stream(I2,O).
```

The following constraint ensures that all annotations satisfy the composition rules:

```
:- dep_rule(I,O,R), not valid_dep_path(I,O,R).
```

In ASP the head of the (constraint) rule above is assumed to be false. Thus, if the body is satisfied the constraint fails. To satisfy the constraint, the body must not be true. So, in the constraint above, either there does not exist a dependency between the input `I` and output `O`, or the dependency forms a valid dependency path. The relation `valid_dep_path(I,O,R)` is true if there is a valid annotation with type `R` between the input `I` and output `O` as defined below.

```
valid_dep_path(I,O,R) :- in(I,P,_), out(O,P,_), dep_rule(I,O,R).
valid_dep_path(I,O,R) :- in(I,P,_), out(O1,P,_), O != O1,
                         dep_rule(I,O1,R1), connected(O1,I1), I != I1,
                         valid_dep_path(I1,O,R2), compose(R1,R2,R).
```

The `connected(O,I)` relation is true if the output `O` shares a data block with the input `I` (implying two program blocks share a dataflow connection from `O1` to `I1`):

```
connected(O,I) :- out(O,_,D), in(I,_,D).
```

The `compose(R1,R2,R)` relation implements the basic dependency composition rules defined in the previous section:

```
compose(R1,R2,R1) :- weaker(R1,R2).
compose(R1,R2,R2) :- weaker(R2,R1).
```

The `weaker(R1,R2)` relation encodes the "strength" of dependency ordering over types (i.e., the $\preceq$ relation; see Section 3). Thus, `weaker(R1,R2)` is true for types `R1` and `R2` iff `R1` $\preceq$ `R2`. The two `compose` rules select the weaker relation of `R1` and `R2`. If `R1` is weaker than `R2`, then the first `compose` rule selects `R1`, and if `R2` is weaker than `R1`, then the second `compose` rule selects `R2`. Finally, the first rule of `valid_dep_path` considers the case where the path is a single program block, and the second rule considers the case where a path consists of multiple program blocks. For the the second `valid_dep_path` rule, we require `O` and `O1` as well as `I` and `I1` to be different values, respectively, for the case where `I` and `O` form a simple cycle. Without the inequalities, checking `valid_dep_path` for `I` and `O` would require `valid_dep_path` for `I` and `O` to be already known (from the body of the rule). We note that workflow cycles, however, are supported by the rules. The following constraint ensures that annotations are the "strongest" along multiple program-block paths.

```
:- dep_rule(I,O,R), valid_dep_path(I,O,R1), R != R1, weaker(R,R1).
```

The constraint ensures there is not a stronger type between the input `I` and output `O` than the one given (guessed or inferred) by the annotation `dep_rule(I,O,R)`.

5 Related Work

We focus on the PROV model, data provenance, and other workflow-based approaches:

The PROV model [12] defines a general *wasInfluencedBy* relationship with *wasDerivedFrom* as the main lineage relationship between entities. PROV also defines subtypes of *wasDerivedFrom*, including *wasRevisionOf*, *wasQuotedFrom*, and *hadPrimarySource*. Although *DependsOn* and *DerivedFrom* are similar to *wasInfluencedBy* and *wasDerivedFrom*, because our approach is designed for computation via workflows, we adopt the more specific notions of dependency (i.e., control and data dependence) from [3]. Our approach is also similar to PROV-O [14], which models provenance at the schema level. We also consider compositions of dependency annotation types, which are not considered within PROV-O.

Cui and Widom [4] define three types of transformations for ETL workflows—dispatchers, aggregators, and black-boxes—and for each a set of techniques for inferring data-level lineage. They also define a number of specialized (i.e., a hierarchy of) transformation types for computing data lineage. While our approach also provides dependency types for transformations (in our case, program blocks), the focus in [4] is to compute data-level workflow lineage (the input items that contributed to output items), and does not consider the differences between dependency, derivation, and so on. The approach used in LabelFlow [1] is also similar to that in [4], in which different types of workflow steps are considered and used for data annotation propagation (i.e., arbitrary metadata attribute-value pair "labels"). Like [4], LabelFlow focuses on workflow execution by inferring data-level labels for intermediate and final workflow data products.

Cheney *et al.* [3] employ dependency analysis techniques (program slicing), which are focused on calculating data dependencies to infer "dependency provenance" for a query language based on the nested relational calculus. Unlike other approaches for inferring lineage from queries, [3] employs dependency analysis to formalize the notion of lineage relationships. Huq *et al.* [9] describe a tool to compute data-level lineage for workflows defined as Python scripts using Program Dependence Graphs (PDGs) [7]. However, control dependencies are converted to data dependencies to simplify lineage relationships for scientists. PDGs are closely aligned with program slicing techniques, and offer a formal interpretation of dependency also adopted by our model.

In [6], data dependencies are inferred from scripts and are then connected to YesWorkflow specifications; a prototype linking YesWorkflow models and noWorkflow traces has been described in [13]. Our approach differs from, but complements these approaches by explicitly supporting lineage assertions for both control and data dependency information (among other types of dependencies) for workflow specifications and enables validation and inference procedures over lineage annotations.

6 Conclusion and Future Work

This paper defines provenance dependency types for modeling lineage constraints within scientific workflow specifications along with a reasoning framework that can validate dependency annotations and infer a complete set of annotations for workflow specifications, including the allowable choices (*possible worlds*) when multiple annotation types are possible. We plan to extend YesWorkflow [11], which uses annotations to declare workflow specifications for executable scripts, with dependency annotations and the reasoning framework described here. We also plan to develop support for annotating subworkflows within YesWorkflow. While the dependency types described here cover a wide range of cases, additional types may be needed for some workflows. For instance, although not described in this paper, we have recently developed extensions for supporting a *NotFlowsFrom* dependency type, which is needed in some subworkflows to capture cases where subworkflow inputs are not connected (i.e., not "up-stream") from subworkflow outputs. Adding *NotFlowsFrom* required only minimal changes to the rules presented in Section 4. Finally, we also intend to explore using static dependency annotations in YesWorkflow models to infer trace-level (runtime) data lineage relationships, thus combining our prior work in [2] with the reasoning framework presented here.

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References

1. Alper, P., Belhajjame, K., Curcin, V., Goble, C.: LabelFlow framework for annotating workflow provenance. Informatics 11(5) (2018)
2. Bowers, S., McPhillips, T.M., Ludäscher, B.: Declarative rules for inferring fine-grained data provenance from scientific workflow execution traces. In: IPAW. pp. 82–96 (2012)
3. Cheney, J., Ahmed, A., Acar, U.A.: Provenance as dependency analysis. Mathematical Structures in Computer Science 21(6), 1301–1337 (2011)
4. Cui, Y., Widom, J.: Lineage tracing for general data warehouse transformations. The VLDB Journal 12(1), 41–58 (2003)
5. Davidson, S.B., Freire, J.: Provenance and scientific workflows: challenges and opportunities. In: SIGMOD (2008)
6. Dey, S.C., Belhajjame, K., Koop, D., Raul, M., Ludäscher, B.: Linking prospective and retrospective provenance in scripts. In: TaPP (2015)
7. Ferrante, J., Ottenstein, K.J., Warren, J.D.: The program dependence graph and its use in optimization. ACM Trans. Program. Lang. Syst. 9(3), 319–349 (1987)
8. Gelfond, M., Kahl, Y.: Knowledge Representation, Reasoning, and the Design of Intelligent Agents: The Answer-Set Programming Approach. Cambridge University Press (2014)
9. Huq, M.R., Apers, P.M.G., Wombacher, A.: ProvenanceCurious: a tool to infer data provenance from scripts. In: EDBT. pp. 765–768 (2013)
10. Ludäscher, B., Bowers, S., McPhillips, T.: Scientific Workflows. In: Encyclopedia of Database Systems, pp. 2507–2511. Springer, Boston, MA (2009)
11. McPhillips, T., Song, T., Kolisnik, T., Aulenbach, S., Belhajjame, K., Bocinsky, R.K., Cao, Y., Cheney, J., Chirigati, F., Dey, S., Freire, J., Jones, C., Hanken, J., Kintigh, K.W., Kohler, T.A., Koop, D., Macklin, J.A., Missier, P., Schildhauer, M., Schwalm, C., Wei, Y., Bieda, M., Ludäscher, B.: YesWorkflow: A User-Oriented, Language-Independent Tool for Recovering Workflow Information from Scripts. Intl. J. of Digital Curation 10(1), 298–313 (2015)
12. Moreau, L., Missier, P.: PROV-DM: The PROV Data Model. W3C recommendation, W3C (Apr 2013), http://www.w3.org/TR/2013/REC-prov-dm-20130430/
13. Pimentel, J.F., Dey, S., McPhillips, T., Belhajjame, K., Koop, D., Murta, L., Braganholo, V., Ludäscher, B.: Yin & Yang: Demonstrating Complementary Provenance from noWorkflow & YesWorkflow. In: IPAW. pp. 161–165 (2016)
14. Sahoo, S., Lebo, T., McGuinness, D.: PROV-O: The PROV Ontology. W3C recommendation, W3C (Apr 2013), http://www.w3.org/TR/2013/REC-prov-o-20130430/