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MASTER THESIS



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Schematron Schema Inference

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I would like to thank to my supervisor, RNDr. Irena Mlýnková, Ph.D., for her guidance, helpful suggestions, study materials and the time she spend reading and correcting my English. It helped me a lot.

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Abstrakt: XML je populární jazyk pro výměnu dat. Mnoho dokumentů však nemá svůj popis schématu nebo je tento popis neaktuální. Tato práce navazuje na práce o automatickém odvozování schémat XML dokumentů a zaměřuje se na odvozování schémat pro Schematron.

Schematron je jazyk, který validuje XML dokumentu pouze pomocí pravidel, ne jako celou gramatiku, jako je typické pro DTD nebo XML Schema. Jelikož oblast generování schémat Schematronu není příliš prozkoumaná, tato práce analyzuje základní problémy, navrhuje několik postupů a popisuje jejich výhody a nevýhody.

Klíčová slova: XML, XML schéma, Odvozování XML, Schematron

Title: Schematron Schema Inference

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Abstract: XML is a popular language for data exchange. However, many XML documents do not have their schema or their schema is outdated. This thesis continues on the field of automatic schema inferring for set of XML documents and focuses on Schematron schema inferring.

Schematron is a language that validates XML documents with rules, it does not compare the document against a grammar like DTD, and XML Schema does. Because the field of Schematron schema generation is not so much explored, this thesis analyzes basic problems, suggests several approaches and describes their advantages and disadvantages.

Keywords: XML, XML schema, XML inferring, Schematron

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1 Introduction

1.1 Motivation

In the current world communication holds a very important role. In the computer world if two entities want to communicate they can accomplish it in many formats.

One of the mostly used is the Extensible Markup Language (XML) [9].

XML is used in many areas and for many purposes and often between different subjects. Each XML document can have a different structure. To express the structure and validate a document against it, XML schema languages were created. Just to name some of them — DTD[9], XML Schema[12] and Relax NG[3]. These schema languages describe the structure of a valid XML document and thus allowing a safe data exchange.

The use of XML schemas is not mandatory and even if they exist, they can outdate real fast. The problem emerges – how to automatically create an XML schema for a set of documents. There have been many works on this problem. But most of them focused on creating a complex grammar. These complex grammars validate the whole document from its root to every leaf. This kind of validation is often slow and also not needed.

What if we want to split the validation into several steps? In each step check a different aspect of the document? What if we want to validate only a specific construct and leave the rest of the document unchecked? These demands were not easily satisfied. Rick Jellife created in 1999 a new schema language for XML validation – Schematron. It uses rules that are able to check only specific parts of an XML document. Schematron is distinct to grammar based schema languages and the ability to automatically generate its schema would be interesting.

1.2 Description of this thesis

In this thesis we will introduce a method to infer a Schematron schema from a set of XML documents. We analyze different aspect of Schematron schema generation. Since the automatic inferring of XML documents is not a new problem, we will

introduce only a single method that we will use in our experimental implementation.

In our experimental implementation we generate a grammar using the introduced inferring method. We allow the user to modify the grammar. The grammar is then transformed into Schematron schema by the use of our algorithm.

1.3 Structure of the work

This chapter presented a motivation and a brief description for this thesis. In Chapter 2 we introduce used technologies (XML, grammar languages, etc.). In Chapter 3 we define formalisms from the language theory. The expressive power of schema languages is compared in Chapter 4. Chapter 5 is the core part of this thesis presenting an analysis and algorithms for Schematron schema generation. Chapter 6 analyzes XML schema inferring and introduces a single method. In Chapter 7 we describe our experimental implementation and its results. Chapter 9 contains summary and also suggestions for possible future work that could not be done in this thesis. The last part of this thesis is the Appendix that contains a brief user guide.

Used technologies

In this chapter we introduce current technologies that are compared and referenced later in this thesis. These descriptions introduce the technologies only in main features. It is not the aim of this thesis to provide the full definition of these technologies.

2.1 XML

In this chapter we define what XML, XML validation and a schema language is. The Extensible Markup Language (XML) is a text-based language standardized by the W3C¹. XML was derived from SGML [14] that was too complex and thus too difficult to implement. XML is simpler but preserves the expressive power. For full definition of XML please refer to [9].

XML is used to describe structured information. XML is a meta-language; it defines only the syntax how to describe the information but not a concrete way how to do it. XML is used in many places for many purposes: sharing data (between people, between programs), communication (e.g. WSDL²), storing data ...

2.1.1 Syntax

XML syntax is easy. Here we define basic terms. To full definition of XML, please see [9]:

Definition 2.1.1. **Tag** is a markup construct that begins with "<" and ends with ">". There are three types of tags – a start tag, an end tag and an empty tag. The difference between these tags is the existence and location of the character "/". Start tag has none, end tag has it right after "<" and empty tag has it right before the ">".

There are limitations for characters that are allowed in the tag name. For full definition of allowed name please see [9].

¹World Wide Web consortium

http://www.w3.org

² WSDL – Web Service Description Language http://en.wikipedia.org/wiki/WSDL

Definition 2.1.2. **Element** is the building stone of any XML document. It begins with a start-tag and ends with a corresponding end-tag or it consists only of a single empty-tag. The names of the tags must match and is case-sensitive. The data (if any) between the start-tag and end-tag is called the **content** of an element. The content can be text or other elements or both. These elements are called **child elements**.

Example 2.1.1. XML markup example

```
<paragraph style="normal">
    Here starts some text. <bold>This part is Important!</bold> <newline />
    Some more text on the next line.
</paragraph>
```

Example 2.1.1 contains three elements: paragraph, bold and newline. Elements bold and newline are within the content of the element paragraph and thus they are child elements. Element newline is formed only of empty-tag and has no content.

Definition 2.1.3. **Attribute** is a name-value pair located within a start-tag or an empty-tag. The value must be always quoted.

Example 2.1.1 contains one attribute *style* that is located in the start-tag of the element *paragraph*. The attribute *style* has the value "normal".

Definition 2.1.4. An XML document is **well-formed** if it contains exactly one root element and all elements are terminated within their parent element's content. (They must be correctly nested)

Example 2.1.2. Not a well-formed document

Example 2.1.2 is not well-formed because elements A and B are not correctly nested.

Note that the order of elements is generally significant; on the contrary the order of attributes of an element is not.

Definition 2.1.5. An XML document is **valid** if and only if it is well-formed and meets some other constraints. These constraints are defined by a **schema language**. The process of determination whether the document is valid is called **validation**.

Example 2.1.3. Well-formed XML document

We can see an example of a well-formed document. The root element is doc, it has two child elements called para that have mixed content of text and element bold (that can be seen in the first paragraph).

2.1.2 Namespaces

Some XML documents have their content from multiple sources – some elements belong to a group A, other elements to group B. As the result the names of elements (or attributes) can collide. Each group has its own schema and we need to determine what schema to use for validation of every specific element. That is the situation where namespaces are used.

Definition 2.1.6. **Namespace** is a context that holds information (e.g. schema) for logically connected data.

Definition 2.1.7. Let us have a namespace NS. Declaration of such a namespace for an element and its content is done using an attribute in the following syntax:

xmlns:NS="URI"

where URI³ points to the namespace declaration. **Default namespace** is defined by setting a value to the attribute xmlns="URI"

A single element can contain definition for several namespaces. See the Example 2.1.4.

Example 2.1.4. Namespace definition

The Example 2.1.4 defines two namespaces — default (http://www.some.examle.com) and namespace sch that points to http://purl.oclc.org/dsdl/schematron.

Definition 2.1.8. Let us have defined a namespace NS. To assign an XML element to that namespace we prefix the name of the element with the namespace. To explicitly set the namespace of an attribute we prefix the attribute's name.

Example 2.2.1. Prefixed element with a namespace

```
<ns1:some-element xmlns:ns1=" http://www.some.examle.com">
    <!-- content of the element with defined namespace ns1 -->
    </ns1:some-element>
```

In Example 2.2.1 we have an element some-element that belongs to the namespace ns1. Namespace ns1 is defined in this element. This namespace is accessible from this element and its content.

6

³ URI – Uniform Resource identifier <u>http://en.wikipedia.org/wiki/URI</u>

2.2 XPath

XPath (XML Path language) [6, 7] is a query language for XML. XPath serves to address parts of an XML document, allowing navigation in the XML document and mining values of element, their attributes, etc. XPath is widely used by other languages and tools (XSLT, XQuery ...). Here we introduce the basics of XPath – syntax, XPath-axis and some of its functions.

2.2.1 Syntax

Here we introduce the syntax of XPath 1.0, its queries and how they are evaluated. An XML document is represented as a tree, where the root node of the tree is the XML document itself and the root node has only one child – the root element of the XML document.

Definition 2.2.1. An XPath **node** is the smallest XML fragment addressable by XPath.

There are several types of XPath nodes:

- Root nodes
- Element nodes
- Text nodes
- Attribute nodes
- Nodes for comments, processing instructions, namespaces...

Each XML document has only one root node and, as mentioned above, it is pointing to the document itself. An element node represents an element in an XML document but not its content. A text node represents the text content of an element's content model (The text is concatenated from each text node that is located in the content model of the element). An attribute node represents element's attributes.

Definition 2.2.2. An XPath **axis** is a relation that specifies what nodes will be selected from a current context.

There are several types of axes which are listed below. For each description of an XPath axis we suppose we have selected a context node U that expresses the relative position.

- **Self** returns the current node *U*.
- **Parent** returns the parent node of *U*.
- Ancestor returns all ancestors of *U*. (All nodes that are present on path from *U* to the root node, excluding *U*)
- Ancestor-or-self returns the result of ancestor axis plus U.
- **Child** returns direct child nodes of *U*.
- **Descendant** returns all descendants of *U*, excluding *U*.
- **Descendant-or-self** returns descendants of *U*, including *U*.
- Preceding-sibling returns all siblings (elements that have the same parent element) that precede *U* in the XML document.
- Preceding returns all elements that precede *U* in the XML document, excluding the ancestors of *U*.
- **Following-siblings** returns all siblings (elements that have the same parent element) that follow *U* in the XML document.
- **Following** returns all nodes that follow *U* in the XML document, excluding the descendants of *U*.
- Attribute selects the attributes of U.
- Namespace selects the namespace nodes of *U*.
 - *Definition 2.2.3. Node test tests the type or name of a node.*
 - Definition 2.2.4. **Predicate** allows for specifying more complex conditions for a node. It is written in square parenthesis and allows using of negation (**not**), **and** and **or** operators.

Predicate can contain another XPath query and (or) use some of the built-in functions of XPath. (e.g. count, location, position...)

Example 2.2.2. Predicate example

[1] - selects the first node from node set

```
[child] – has a child element "child"
[@id = 500] – has an attribute "id" with a value of 500.
```

Definition 2.2.5. **Location step** is a function that returns a set of nodes. It has the form of:

axis::node-test predicate1 predicate2 ... predicateN,

where axis is an XPath axis and it is optional, the default axis is the child axis, node-test is required and predicates are optional. If the axis is omitted the double-colon is also omitted.

Example 2.2.3. Examples of location steps

child::book[count(para) > 1]

Example 2.2.3 returns all children of the current node that have the name book and each returned book must have at least one child element para.

Definition 2.2.6. **Location path** is a sequence (can be empty) of location steps concatenated with "/".

Location path is sometimes called **path** or **query**.

Definition 2.2.7. **Absolute location path** is a location path that begins with a "/". The context for absolute path is always the root node.

Example 2.2.4. Absolute location path

/ - absolute path that selects only the root node (no location steps)

/* - selects all children of the root node – document root (there is always only one document root)

In Example 2.2.4 the second path selects any child node of the root node. The asterisk (*) select any node that has a name. Each element or attribute has a name.

Definition 2.2.8. **Relative location path** is a location path without "/" at the beginning. Relative path must have specified a context set of nodes.

Example 2.2.5. Relative location path examples

Let us use Example 2.1.3 (Well-formed XML document), let the context node be the root element "doc". The following relative location path

para/bold/text()

would return the text node (the text) of the element bold that is the child of element para that is the child of the context node.

```
descendant::bold/parent::para
descendant::para[bold]
```

Both paths return the element para that has a child element bold.

XPath abbreviations

The mostly used axes have their abbreviations.

- Child <-> /
- Descendant-or-self::node()/ <-> //
- self <->.
- parent::node() <-> ..
- attribute <-> @

Example 2.2.6. Example of abbreviations

```
/doc <-> /child:doc
bold/.. <-> bold/parent::node()
//bold <-> /descendat-or-self::node()/bold
```

2.2.2 XPath 2.0

The next version of XPath – version 2.0 brings new features like data types, more built-in functions, ordered sequences and regular expressions [8]. Due to space limitations it is left to the reader for his or her interests to read [8] for more information.

2.3 DTD

The Document Type Definition (DTD) is a schema language. It allows to define constrains for SGML family of languages and contrary to later schema languages it does not use XML. It describes the constraints for every element and its content [9]-Chapter 2.8.

Example 2.3.1. A DTD example

```
    <!DOCTYPE document [</li>
    <!ELEMENT title (#PCDATA) >
    <!ELEMENT paragraph (#PCDATA | bold | newline)* >
```

- 4. <!ELEMENT bold (#PCDATA) >
- 5. <!ELEMENT newline empty>
- 6. <!ATTLIST paragraph style CDATA #implied >
- 7.]:

Example 2.3.1 is a short DTD definition for an XML document. Example 2.1.1 contains a possible XML fragment of such a document.

Each DTD starts with the markup "<!DOCTYPE " followed by the name of the root element (In the Example 2.3.1 *document*). Each element that occurs in the content of the root element must be listed before the closing markup "]>".

Definition 2.3.1. A **pattern** describes the allowed content model. Pattern is built from other patterns and from basic structures of a validation language. (e.g. attributes, elements). A pattern of an element is a definition of the allowed content model of this element.

Elements (including the root element) are defined by the markup "<!ELEMENT" followed by the name of the element and its pattern and at last closed by the markup ">".

The content of an element can be element or text data. Text data are marked as "#PCDATA" (line 2 in Example 2.3.1). If the element should be empty, it is defined as "empty" (line 5). Empty definition cannot be combined. Other types of content can be combined with each other using several operators: Operator choice (|) and sequence (,) and quantity operators zero-or-one (?), zero-or-many (*) and one-or-many (+).

At line 3 of Example 2.3.1 we can see that the element paragraph can contain of any combination of text data, element bold and newline in any quantity.

2.4 XML Schema

XML Schema [12] is a schema language that evolved over the past few years. Version 1.0 of the language has been published in 2001 by the W3C. In 2009 a new candidate version (1.1) has been published [13]. This definition of XML Schema definition language uses the abbreviation XSD. This abbreviation is also sometimes used for a XML Schema definition in the meaning of a schema document instance of

the XML Schema. If not said otherwise we will use the XSD as the abbreviation of XML Schema Definition Language.

In this thesis we work with version 1.0 of XSD. Nowadays it is one of the most commonly used schema languages. It was created because DTD was not strong enough (bad support for foreign keys, missing data types and namespaces...) but there are many principles that are similar to DTD.

2.4.1 Syntax

XSD defines the allowed content of an XML document based on defining parentchild relationship. It defines the allowed content for the root element and its attributes. Recursively defines the child elements of root and their children.

Definition 2.4.1. XSD file is an XML document with the root element schema and the namespace "http://www.w3.org/2001/XMLSchema".

Data types

XSD supports many built-in data types (e.g. boolean, int, double, date, string...) and allows for defining user-defined types as well. There are two types of data types in XSD - simple and complex data types.

All embedded XSD types are **simple types**. A user can create new simple types using extension or restriction of another simple type or just by defining a list of allowed values. Simple types are used to store simple values like text, amount of money, post code... but not a structured data – elements or attributes. For that purpose complex data types are used.

Example 2.4.1. Simple types in XSD

In Example 2.4.1 we define a simple type for the post code of an address. It is based on string and we limit its length to 5 characters.

Complex data types are used to store a complex (structured) element content – containing multiple elements and (or) attributes. A child element may be defined directly in the definition of its parent element. It is also possible to define its exact occurrence by using **minOccurs** and **maxOccurs** attributes. An item can be made optional by setting minOccurs to "0".

There are generally three options to define complex types: deriving from a simple type (we use simple type with attributes), from a complex type or defining a new complex type. Deriving from an existing data type is done via extension or restriction. For purposes of this thesis we show the definition of a brand new complex type.

Defining the pattern for a complex type is done with pattern operator **sequence**, **choice** or **all**. These operators control the order of their patterns.

- Operator sequence ensures that child patterns are validated against the order they are listed in their definition. The content of this operator is limited to pattern element, sequence and choice.
- Operator choice selects only one pattern from its child patterns. The content
 of this operator is limited to pattern element, sequence, choice and all.
- Operator all validates its pattern in any order. The occurrence of patterns can be set to at most once. This feature is not directly in DTD, but it can be still expressed by a more complex pattern definition. However the content of this operator is limited only to elements (Chapter 3.8.2 in [12] also note the containts in Chapter 3.9.6). These constraints ensure a deterministic data model.

Example 2.4.2. Complex type example

In Example 2.4.2 we define a pattern for element "person". The pattern consists of a sequence of elements firstName, optional middleName and lastName and a choice of elements passportNo and IDCardNo.

2.4.2 Summary of XSD

XSD allows for complex definition of a schema for an XML document. It supports more user friendly features like "all" operator or better support for foreign keys, and data types. As we will see in Chapter 4, the expressive power of XSD is stronger than of DTD. Some features of XSD are merely a syntactic sugar (like the operator all).

2.5 RELAX NG

RELAX NG [3] is another schema language. It was created by merging two former schema languages — RELAX CORE [15] and TRex [16]. RELAX NG language has a strong mathematical background. Its schemas can be written in two forms: XML or "compact"; these two forms can be translated to each other without the loss of important information. In this chapter we will introduce the basic aspects of XML syntax of RELAX NG.

2.5.1 XML Syntax

RELAX NG has similar syntax as XSD, but as we will see in Chapter 4, that RELAX NG is stronger than XSD. It also supports namespaces.

Example 2.5.1. RELAX NG simple example

```
<element name="addressBook">
     <zeroOrMore>
     <element name="card">
```

```
<choice>
<element name="name">
<text/>
</element>
</choice>
<element name="email">
<text/>
</lement>
</element>
```

In this example we define pattern for element "addressBook". It contains zero or more elements "card". Each "card" contain either element "name" or element "email".

Elements are defined using the element **element**. Their pattern is defined by patterns below.

- element
- attribute
- group
- interleave
- optional
- choice
- zeroOrMore
- oneOrMore
- data types

Group pattern connects its child patterns in serial order. *Interleave pattern* on the contrary allows its child patterns to be in any order (with no limitation to the child patterns) but every pattern must be present. **Optional pattern** allows a pattern to be omitted. **Choice pattern** selects only one of its child patterns. **ZeroOrMore**

pattern repeats zero or more times. **OneOrMore pattern** repeats one or more times.

RELAX NG supports data types like XSD does. In fact, it allows the usage of data types from XSD and their parameterization.

Name classes

Both the DTD and XSD allow the definition of elements only by specification of a name or type (in case of XSD). They are unable to define schema like "The root element can have only this pattern regardless its name" because in the schema we do not know the name (or type) of the root element and we do not want to define it.

RELAX NG has a feature called "name classes". This feature allows for defining elements and attributes anonymously or with some restrictions. Normally we would use the **name** attribute or element. To define a pattern for more than a single name we do not give elements (or attributes) their name but we use one of following elements specifying their name class:

- anyName
- nsName
- choice

Construct **anyName** defines that the element (or attribute) can have any name. It can be restricted by **nsName** or **name** elements, see Example 2.5.2. There we define an element that can have any name except for name "root" and must not have the default namespace.

Example 2.5.2. anyName name class example

```
<!—more definition of content -->
</element>
```

In Example 2.5.2 we define a name class for an element pattern. The element can have any name from non-default namespace except the name root.

Construct **nsName** specifies the allowed namespace for a name. Again the namespace can be restricted by an element **except**. Choice (in context of name class) allows combining of previous options.

Example 2.5.3. nsName name class example

```
<element>
<nsName ns=" http://www.someNameSpace.com">
<except>
<name>root</name>
</except>
</nsName>
<!—more definition of content -->
</element>
```

The allowed name for Example 2.5.3 is any name, except the name root, from the namespace "http://www.someNameSpace.com".

Example 2.5.4. choice name class example

In Example 2.5.4 we define three possible options for name of this pattern — "root", "document" or the default namespace.

Definition 2.5.1. **Co-constraint** or **Co-occurrence** constraint is a set of rules that control what markup (elements or attributes) can co-occur together. [5]

RELAX NG allows for expressing some co-constraints, mainly in the parent-child relationship. See Example 2.5.5. There we define pattern for contact. We allow for storing two kinds of contacts - email or phone. On the basis of the value of attribute "type" we control the inner markup.

Example 2.5.5. Co- constraint example

```
<element name="contact">
    <choice>
           <group>
                 <attribute name="type">
                        <value type="string">email</value>
                 </attribute>
                 <element name="emailAddress">
                        <text />
                 </element>
           </group>
           <group>
                 <attribute name="type">
                        <value type="string">phone</value>
                 </attribute>
                 <oneOrMore>
                        <element name="phoneNumber">
                              <text/>
                        </element>
                 </oneOrMore>
           </group>
    </choice>
    <!--other contact definition common for both contact types -->
</element>
```

In Example 2.5.5 we define pattern for a contact element. It depends on the type attribute. If the attribute has value email, the rest of the pattern is only an element emailAddress. If the type is phone then the rest of the pattern is one or more elements phoneNumber.

2.5.2 Summary of RELAX NG

RELAX NG allows for creation of complex schemas that are well readable. The schemas can be written in two forms (XML and compact). RELAX NG has two big

advantages: name classes and co-constraints. Contrary to XML Schema there is another advantage – non-determinism. RELAX NG has stronger expressive power than XSD or DTD.

2.6 Schematron

Schematron is an XML validation language [2]. It defines rules that validate documents by presence or absence of XML patterns. These rules are short, simple and allow for printing user friendly messages.

2.6.1 Versions of Schematron

Schematron was developed by Rick Jellife in 1999. Since then many implementation were created and the language itself evolved. We will describe the most common variants.

Schematron 1.5

Version 1.5 of Schematron was built by Rick Jellife and contains of two-stage XSLT 1.0 transformation. The first transformation transforms a Schematron definition into new XSLT transformations these are then run to validate XML documents. It is easy-to-use but uses only XSLT 1.0 as a query language.

ISO Schematron

Schematron has been standardized by ISO/DSDL [17] project as ISO/IEC 19757-3. It brings new ideas and extends and changes Schematron 1.5. The main differences are support for more query languages, variables, abstract patterns and new URI.

In this thesis we will use ISO Schematron if not stated otherwise.

Schematron 1.6

This version of Schematron is the transition between Schematron 1.5 and ISO Schematron.

2.6.2 Language definition

The syntax for Schematron is fairly easy. A full RELAX NG schema for Schematron can be found at [2]. We will explain here the most important features and constructs.

Schematron understands **namespaces** and thus we can combine Schematron with other namespace-aware schema languages. The namespace definition for Schematron is located on [18].

As said at the beginning of this chapter, ISO Schematron can use different query languages – this means, we can create schemas that query using XSLT 1.0 [19], XSLT 1.1 [20], XSLT 2.0 [21], XQuery [22], XPath [6] or XPath 2.0 [8]. The full list of supported implementations can be found in the ISO Schematron definition and depends on the implementation used. The list of supported query languages of each implementation may differ because new query languages can be supported if they implement a set of rules that corresponds to Schematron definition. The definition of a query language "queryBinding" is located in the element "schema" and can be omitted.

Example 2.6.1. Schematron namespace

In the Example 2.6.1 we define a Schematron schema using Schematron namespace as a default namespace. We also define the query language - XPath2, title of schema and a pattern.

Phases and patterns

Each Schematron schema must have at least one pattern element. Each pattern in Schematron represents a set of rules that are processed. By default every pattern is marked as active and thus processed during validation process. Schematron allows for defining **phases** that change this default behavior. Each phase contains a set of patterns that should be executed. Phases allow for splitting complex validation process into steps or parts. The active phase is defined in a command line or in the schema (attribute defaultPhase).

Example 2.6.2. Schematron phases

Schema definition in Example 2.6.2 contains three patterns (simple_index_validation, word_blacklist and complex_validation) and two phases (simpleValidation and complexValidation). The default phase simpleValidation. If the default phase is selected, it processes the simple_index_validation and word_blacklist patterns.

There are three types of **patterns** in Schematron – normal, abstract and "is-a" pattern. Normal pattern contains a set of rules and if active, it processes them. Abstract pattern also contains rules, but must have specified the attribute abstract="true". They may use undefined variables (they are defined by a caller "is-a" pattern). "Is-a" pattern does not contain any rules. It contains attribute "is-a" with reference to an abstract pattern. They may contain "param" elements that define the values of all undefined variables of the abstract pattern.

Example 2.6.3. Patterns

Example 2.6.3 contains four patterns. The first two are normal patterns. Each defines one rule. The third pattern is an abstract pattern. The last one is a "is-a" pattern.

Rules and assertions

Schematron validation capability is based on its **rules**. Each pattern must contain at least one. Each rule must have a context in which it runs assertions. Schematron contains two types of assertions: positive - **asserts** – and negative - **reports**. If any assertion of the rule fails the rule fails and the document is marked as invalid. Note that as the result of this paragraph Schematron allows for both positive and negative validation.

Definition 2.6.1. An **Assertion**, in the context of XML validation, is a statement about an XML fragment. A **positive assertion** succeeds if the statement of the assertion succeeds. A **negative assertion** succeeds if the statement fails.

Example 2.6.4. Assertions

</Schematron>

In Example 2.6.4 we have a single rule that contains two assertions about every book in the tested XML document. Positive (assert) that checks that every book has an element title. Negative assertion (report) that tests there are no book elements that would contain other book element in its content.

Diagnostic and value-of

Schematron assertions – assert and report – both contain a user-defined text of assertion - Example 2.6.4. This text can be enriched by the construct "value-of". Value-of queries a value in the validated document and returns it. See Example 2.6.5.

Example 2.6.5. Assertions with value-of

In Example 2.6.5 we have changed Example 2.6.4. We added an assert for attribute ID and extended the assert testing the title. Now if the title assert fails it prints the ID of the book that is missing the title.

Sometimes we would need to print the same message repeatedly for multiple assertions, like help. For this purpose we can use the diagnostic construct. Diagnostics generate text and can be referenced from Schematron assertions. If the assertion fails, it prints its message and then it prints the diagnostic. The diagnostic construct can contain the "value-of" construct. Its context is the context of the assertion that called the diagnostic.

Example 2.6.6. Diagnostics

```
<schema xmlns=" http://purl.oclc.org/dsdl/schematron" queryBinding="xpath2">
  <pattern>
         <rule context="//book">
               <assert test="@id" diagnostics=" printHelp">Every book must have an
id</assert>
               <assert test="title" diagnostics=" printHelp">The book with id <value-of
select="@id" /> must have an element title</assert>
                <report test="book" diagnostics=" printHelp">Book cannot have any other
book</report>
         </rule>
  </pattern>
  <diagnostics>
         <diagnostic id="printHelp">
                For more information, see the validation requirements for this document.
www.example.com/documentantation
         </diagnostic>
  </diagnostics>
</Schematron>
```

Example 2.6.6: We have extended Example 2.6.5 with the usage of diagnostics. Each assertion now prints the same help.

Variables and let construct

Schematron allows creating variables and using them in later queries. Schematron variables are created with the let construct.

Let construct contains only two attributes name and value. Name attributes defines the name of variable, the value attribute defines its value. Variables are addressed with their name prefixed with "\$". See Example 2.6.7.

Example 2.6.7. Let construct

Example 2.6.7 shows the usage of let construct. We define a rule and store the count of preceding books. It the book does not have the id attribute, the assertion will contain the position of the book.

Let construct is allowed as a child of schema, phase, pattern and rule. The context for value expression of the let construct is the rule context for rule, or document root otherwise.

2.6.3 Difference from other schema languages

Schematron is not a classical XML validation language (like DTD, RELAX NG or XML Schema) that must define the whole structure of the XML document (regular grammar) they validate. Schematron defines rules for patterns that validate the document - we create only rules we are interested in. The number of these rules can be significantly lower and because of that the whole Schematron document can be smaller. See Example 2.6.9 for example of DTD. In Example 2.6.10 there is a Schematron definition for the same file. Other main advantages of Schematron are that we can define relationships between XML markups (co-constraints) and define rules for general usage (name classes of RELAX NG, but less restricted) See Example 2.6.13 where we create a rule for the root node independently its name.

Example 2.6.8. Book list example – xml fragment

In Example 2.6.8 we have an XML fragment from a book database. This fragment is a part of a bigger XML document. In this example there are three books, each book has an id attribute (values 1, 2, 3) and elements author and title.

Example 2.6.9. DTD definition for the book list

```
<!DOCTYPE books [

<!ELEMENT books (book*)>

<!ELEMENT book (author+, title)>

<!ELEMENT author (#PCDATA)>

<!ELEMENT title (#PCDATA)>

<!ATTLIST book id CDATA #REQUIRED>
]>
```

In Example 2.6.9 there is a DTD definition for xml fragment from Example 2.6.8.

Note that the DTD allows a book element to have more authors, this cannot be anticipated from the fragment we have.

Example 2.6.10. Schematron definition

Example 2.6.10 shows the Schematron definition for the XML fragment of Example 2.6.8. It has only one pattern that contains only one rule. This definition checks only the presence of required attributes, but does not check the order or the occurrence of elements and attributes. It is for the simplicity of this example. Schematron also allows for printing defined assertation messages.

Advantages of Schematron

The real strength of Schematron is the ability to define all kinds of relationships we know from XPath—axes (e.g. "following", "descendant-or-self"). The classical grammar languages are able to define only parent/child and sibling relationships.

Notable features:

Co-constraints: Making a constraint about nodes (XPath) based on a
presence or a value of another node(s). (Element-to-element, attribute-toelement and attribute-to-attribute)

Example 2.6.11: There are two elements min and max. We define that the value of element min must be lower than or equal to the value of element max.

Example 2.6.12: If there is an attribute A, the parent element must be C or D otherwise.

- Making general constraints for elements (like name classes in RELAX NG, but stronger).
 - Example 2.6.13: The root element must have a specific form in this example a date attribute. If the document is valid, the date information is printed.

 (Note that we do not need to know what the name of the root element is.)
- An author of a Schematron schema writes his own messages for asserts. This
 is an advantage during validation as it allows explaining the error and can
 give hints for correction.

Example 2.6.11. Co-constraints example

In this example we check values of two elements – min and max.

Example 2.6.12. Parent element check example

```
</rule>
</pattern>
</schema>
```

Here we define that each element that is not a root element and has an attribute A must have a parent element C. If it does not have the attribute A, the parent element must be D. An example of an invalid XML file and the result of validation follow.

```
<?xml version="1.0" encoding="utf-8"?>

<D>

<C>

<some-element-without-A />

<element-with-A A=" "></element-with-A>

</C>

<any-element-without-A />

<bad-element-with-A A="should not be here" />

</D>
```

This file is not valid and contains two errors:

- /D/C/some-element-without-A: The only allowed parent element for an element without attribute "A" is element "D".
- 2. /D/bad-element-with-A: Only element "C" can have a child element with attribute "A".

Example 2.6.13. General root constraint example

In Example 2.6.13 we check the existence of attribute date in the root element. We accept only date as element, if it should be presented as an element, we report it as well.

Disadvantages of Schematron

The language is relatively young and is still evolving. There are many implementations and versions; however thanks to the standardization of ISO Schematron, this should be solved.

The Schematron is not suitable for defining and checking the whole structure of an XML document, mainly the order or cardinality of elements. (We mean the construct "sequence" from XSD or "group" from RELAX NG.) For this purpose it is recommended to use a grammar language like RELAX NG, XML Schema or DTD. Note that Schematron definitions can be placed into XSD or RELAX NG schema and thus enhances the validation capability of that validation language. In Example 2.6.14 we show an example of a Schematron definition in an XSD schema (Version 1.0). Schematron definitions are placed in the "appinfo" element. Please note that version 1.1 of XML Schema allows for defining its own constructs of asserts. In this thesis, we consider only XML Schema of the version 1.0.

Example 2.6.14. Schematron within XML Schema 1.0

```
<?xml version="1.0"?>
<xsd:schema xmlns:xsd="http://www.w3.org/2001/XMLSchema"
targetNamespace="http://www.demo.org"
xmlns="http://www.demo.org"
xmlns:sch="http://purl.oclc.org/dsdl/schematron"
elementFormDefault="qualified">
     <xsd:annotation>
           <xsd:appinfo>
                  <sch:title>Schematron validation</sch:title>
                  <sch:ns prefix="d" uri="http://www.demo.org"/>
           </xsd:appinfo>
    </xsd:annotation>
     <xsd:element name="Limits">
           <xsd:annotation>
                  <xsd:appinfo>
                        <sch:pattern">
                               <sch:rule context="d: Limits">
                                     <sch:assert test="d:max > d:min"
diagnostics="lessThan">MAX should be greater than MIN.</sch:assert>
                               </sch:rule>
```

```
</sch:pattern>
                        <sch:diagnostics>
                               <sch:diagnostic id="lessThan">Error! Max is less than Min.
Max = <sch:value-of select="d:max"/>
Min = <sch:value-of select="d:min"/>
                               </sch:diagnostic>
                        </sch:diagnostics>
                  </xsd:appinfo>
           </xsd:annotation>
           <xsd:complexType>
                  <xsd:sequence>
                        <xsd:element name="min" type="xsd:integer"/>
                        <xsd:element name="max" type="xsd:integer"/>
                  </xsd:sequence>
           </xsd:complexType>
    </xsd:element>
</xsd:schema>
```

This example connects XML Schema with Schematron schema. We extend the Example 2.6.11.

3 Basic Definitions

In this chapter we introduce basic definitions that are used later in this thesis. The definitions are taken from theoretical computer science, Language and Automata theory. After the basic definitions we formally define regular expressions that were more or less used in the previous chapter and will be used more in this and later chapters. Later on we introduce definitions for hedges and regular tree automata and grammars. At the end of this chapter we define subclasses of regular tree languages. This chapter is based on [1], [10], [11] and [23].

3.1 Formal Languages Theory

In this chapter we introduce the basics of language theory and regular trees. We start with basic terms like alphabet, word, language and grammar and introduce the Chomsky hierarchy.

3.1.1 Basic definitions

Definition 3.1.1. An **alphabet** Σ is any finite set of symbols (or letters). Finite sequence of symbols over an alphabet Σ is called a **word**. Empty word is denoted by λ .

The set of all words over an alphabet Σ is denoted by Σ^* .

Definition 3.1.2. A formal language **L** *over an alphabet* Σ *is a subset of* Σ^* .

A formal language can be defined in several ways: set of words, or by some formalism like grammar, regular expression or an automaton.

Example 3.1.1. Example of an alphabet, word and a language

Let us have $\Sigma =$ all small letters. (That is informally written $\Sigma =$ [a-z]).

A word over the \sum can be "hi", "a", "aab", or any other combination of letters from this alphabet.

We can define language L to be a set of words {a, ab, abb, abbb, ...}

Definition 3.1.3. Let us have a word $w \in \Sigma$ and $i \in N$, the i-th **power** of a word w. We denote w^i as a sequence $www \dots w$. More formally power is a function P(w,i), defined as: $P(w,0) = \lambda$ P(w,1) = wP(w,n) = wP(w,n-1)

Example 3.1.2. Power of words

```
a^{2} = aa
(ab)^{3} = ababab
ba^{5} = baaaaa
```

Example 3.1.2 shows the usage of the power function and the result of applying it to three words.

Definition 3.1.4. A formal grammar G is tuple G=(N, T, S, P), where N is a finite set of non-terminal symbols, $T \in \Sigma$ is a finite set of terminal symbols that is disjoint from $N, S \in N$ is the starting non-terminal and P is a finite set of production rules of the form $(N \cup T)^*N(N \cup T)^* \rightarrow (N \cup T)^*$

Definition 3.1.5. The language of a formal grammar G=(N, T, S, P), denoted as L(G), is a set of all words over \sum that are generated by repeated application of production rules to S until there are no non-terminal symbols left.

Example 3.1.3. Production rule

Let us have grammar G1 = (N1, T1, S, P1), where N1 = {S, A, B}, T1 = {a, b} and P1 contains the following production rules: $S \rightarrow A \mid B$ $A \rightarrow a \mid aB$ $B \rightarrow b \mid bB$ The generated language L(G1) = {a, b, ab, bb, abb, bbb,...}.

Example 3.1.3 shows a definition of grammar G1 and the language L(G1).

Chomsky Hierarchy

Chomsky Hierarchy[23] classifies formal grammars into four categories based on the complexity of production rules they use. The higher the category is, the stricter the production rules are.

- Type 0 unrestricted grammars include all formal grammars from Definition 3.1.4. They generate exactly all languages that can be recognized by a Turing machine.
- Type 1 context-sensitive grammars have production rules of the form:
 aXb → axb, where a,b ∈ (N U T)*, x ∈ (N U T)+ and X ∈ N. The rule S → λ is
 allowed only if the non-terminal S does not appear on the right side of any
 production rule. These formal grammars generate context-sensitive
 languages.
- Type 2 context-free grammars have production rules of the form: $X \rightarrow w$, where $X \in \mathbb{N}$ and $w \in (\mathbb{N} \cup \mathbb{T})^*$. They generate context-free languages.
- Type 3 regular grammars have production rules of the form: $X \to xY$ or $X \to x$, where $X,Y \in N$ and $x \in T$. The rule $S \to \lambda$ is allowed only if the non-terminal S does not appear on the right side of any production rule. This category of grammars is recognized by a *finite state automaton*. These formal grammars generate regular languages. The regular languages can be also obtained by regular expressions.

3.2 Regular expressions and finite automata

Regular expressions describe a regular language. They have the same expressive power as a regular grammar. We first introduce the definition of regular expressions, some informal examples and, finally, a formal definition of regular expression evaluation is introduced.

Definition 3.2.1. Regular expression R is a sequence over an alphabet $\sum U\{?, *, +, |, (,), ","\}$, where ? is the zero-or-one operator, * is the zero-or-more operator, + is the one-or-more operator, | is the choice operator, | is a sequence operator and | or grouping parenthesis.

The test if a word is described by a regular expression is called *matching*. For regular expression there is often used the abbreviation **regex**. The sequence operator "," is sometimes omitted. E.g. The regex "a,b" equals to "ab".

We can use regular expression for Example 3.1.3 and define the language L(G1) as $L(G1) = (a|b)b^*$.

We now informally describe what each regular expression operator does.

- Grouping parenthesis (,) change the scope of operators. Normally operator
 matches only single preceding (or following) symbol, if there are grouping
 parenthesis then the operator matches the whole content of the
 parenthesis.
- Operator | matches either a preceding or a following symbol.
- Quantity operators ?, * and + specify how often the preceding symbol (or group) can occur.
 - o Operator? zero-times or once.
 - Operator * zero or many times.
 - Operator + one or many times.

Example 3.2.1. Regular expressions

```
R1 = "ab?c" matches {abc, ac}

R2 = "b|c" matches {b, c}

R3 = "abc*" matches {ab, abc, abcc, ...}

R4= "abc+" matches {abc, abcc, abccc,...}

R5 = "a(b|c)+" matches {ab, ac, abb, acc, acb, acc,...}
```

Now we formally describe the evaluation (matching) of regular expression.

We denote the set of all regular expressions R over and alphabet A as RegExp(A). Let us have R, R_1 , $R_2 \in RegExp(A)$ and $a \in A$. The language of regular expression is defined by induction:

• $R = R_1$? $L(R) = L(R_1) \cup \{\lambda\}$ • $R = R_1 +$ $L(R) = \bigcup_{i \in N} \{u^i \mid u \in L(R1)\}$ • $R = R_1 *$ $L(R) = \{\lambda\} \cup L(R_1 +)$ • $R = (R_1)$ $L(R) = L(R_1)$

3.2.1 Non-deterministic finite state automata

In the previous chapter we have showed one way to express the Regular grammars (Type 3 in the Chomsky hierarchy). In this chapter we show a different approach using finite state automata.

Definition 3.2.2. [26] Nondeterministic finite state automaton (NFA) is a tuple $A = (Q, X, \delta, S, F)$ where Q is a finite non-empty set of states X is a finite non-empty alphabet δ is transition function $\delta: Q \times X \to P(Q)$, where P(Q) is the power set of Q $S \subseteq Q$ is the set of starting states and $F \subseteq Q$ is the set of final states.

Definition 3.2.3. [26]We say that a word $w = x_1 x_2 \dots x_n$ is accepted by NFA $A = (Q, X, \delta, S, F)$, if there exists a sequence q_1, q_2, \dots, q_{n+1} that $q_1 \in S$ and $q_{i+i} \in \delta(q_i, x_i)$ for $i = 1 \dots n$ and $q_{n+i} \in F$.

For the later use we define a theorem of automata equivalence. For that we need to define automaton homomorphism.

Definition 3.2.4. [26]Let us have two NFAs A_1 and A_2 . We say that the transition $h: A_1 \to A_2$ is (automaton) homomorphism if and only if: $h(Q_1) = Q_2$, that means $\forall q \in Q_1 \exists p \in Q_2 : h(q) = p \land \forall p \in Q_2 \exists q \in Q_1 : h(q) = p$, $h(\delta_1(q,x)) \to \delta_2(h(q),x)$ and $h(F_1) \iff h(F_2)$.

Here we used transition on a set we define it as follows: $h(Q_1) = Q_2$ means $\forall q \in Q_1 \, \exists p \in Q_2 \colon h(q) = p \, \land \, \forall p \in Q_2 \, \exists q \in Q_1 \colon h(q) = p$.

Theorem 1 Automata equivalence

[26] If there exists automata homomorphism between finite NFAs A_1 and A_2 , then A_1 and A_2 are equivalent.

Proof

Finite iteration

Let us have
$$h(\delta_1(q,w)) \to \delta_2(h(q),w)$$
 and $w \in X^*$ $w \in L(A_1) \iff \delta_1(q_1,w) \in F_1 \text{ for some } q_1 \in S_1$ $\iff h(\delta_1(q_1,w)) \in F_2$ $\iff \delta_2(h(q_1),w) \in F_2$ $\iff \delta_2(q_2,w) \in F_2$ $\iff w \in L(A_2)$

Lemma 1 Each regular expression R can be converted to a NFA A_R so that $L(R) = L(A_R)$.

Proof

There are two ways shown in [26]. We will not show here the whole proof, only the basic idea. For each symbol $s \in R$ we create an elementary NFA (accepting empty or single-letter languages). We merge these elementary NFA based on regex operations. \blacksquare

3.3 Regular tree grammars and Hedges

Now we will define grammar that is used to describe the tree-like documents, such as XML. This chapter is based on [10] and [11].

XML documents are special, they have only one root element. Each element can have multiple children (elements, attributes...). Without any loss of generality, we will now consider that XML document consists only of elements. Attributes, text content, namespaces... can be all considered as special elements with no children. Our simplified XML document is a tree – it has only one root, elements are nodes and leaves.

In literature, regular tree grammars are often used for definition of tree languages. We will introduce here their definition. However, as it may look that XML documents are well expressed with regular tree grammar, we will show later in this chapter, that this is not true. Therefore, we introduce hedges and their grammars and languages.

Definition 3.3.1. [11] A **ranked alphabet** is a couple (F, Arity) where F is a finite set and Arity is a mapping from F into \mathbb{N} . The arity of a symbol $f \in F$ is Arity(f).

A ranked alphabet defines an arity for each symbol. Based on their arity we can call them variables, unary, binary ... n-ary operators. Before we introduce regular tree grammar, we will define term and tree.

Definition 3.3.2. A **term** t over an alphabet A and a set of variables X is defined in the form of: $t := a(t_1, t_2, ... t_n)$, or t := x where $a \in A$ and $t_1, t_2, ... t_n$ are terms over A, n >= 0 and $x \in X$. For ranked alphabet the number n is equal to Arity(a).

We denote set of all terms over an alphabet A and variables X as **Term(A,X)**.

Definition 3.3.3. A **ground term** g over an alphabet A is a term from $Term(A, \emptyset)$. We denote set of all ground terms over A as GroundTerm(A).

Ground term is in fact a term without a variable.

Definition 3.3.4. A **tree** t over an alphabet A is a subset of GroundTerm(A).

We denote set of all trees over an alphabet Σ as $T(\Sigma)$.

Next we introduce the definition of regular tree grammar from [11]. We will use this definition for comparison with hedges.

Definition 3.3.5. [11] **Regular tree grammar** G over ranked alphabet is a tuple (S, N, F, R) where S is a starting symbol, $S \in N$, Arity(S) = 0 N is a finite set of non-terminals over a ranked alphabet F is a finite set of terminal symbols from a ranked alphabet and $N \cap F = \emptyset$ $R: N \to Term(N \cup F \cup X)$, where X is set of variables

Hedges

[10] defines regular tree grammars over an alphabet with infinite arity. [11] contains second definition of regular tree grammars over unranked alphabet. These definitions of tree grammar are sometimes called hedges.

Using ranked alphabet for XML documents is problematic – elements (terminal symbols) must correspond to their arity, but an XML document generally does not limit the number of children of elements. That is the reason we will use unranked alphabet.

An **unranked alphabet** is nothing more than just a normal alphabet defined at the beginning of Chapter 3.

The order of elements in XML may or may not be important. For example for structured data the order is not important, but for an XML document (e.g. XHTML[24]) the order may be important. Let us have an XML document with a root element a and sub trees t_1 , t_2 ... t_n , we can depict the document as $a(t_1, t_2$... $t_n)$. Now comes the question, how to call all the sub-trees of the element a. A set of trees is a forest, but a set does not reflect the order. That is why the term hedge is used. **Hedge** is a **sequence** of trees. Hedges are used for definition of formalism that is connected with XML.

There are many definitions of hedge grammars. We will use the one from [10], there it is called regular tree grammar, but it is also a hedge grammar definition.

Definition 3.3.6. **Regular hedge grammar** *G* is a tuple (N, T, S, P) where:

N is a finite set of non-terminals,

T is a finite set of terminals over an unranked alphabet,

S is a set of start symbols, where $S \subset N$,

P is a finite set of production rules of the form $X \to \alpha r$, where

 $X \in \mathbb{N}$, $a \in T$ and r is a regular expression over \mathbb{N} . X is the left-hand side, a r is the right-hand side, and r is the content model of this production rule.

We abbreviate rules of the form of $X \rightarrow a\lambda$ to the form $X \rightarrow a$. Some definitions of hedges use parenthesis to separate the regular expression from the label (non-terminal). We will use this one.

As said before, hedge grammars are used for unranked ordered trees. An extension for unranked unordered trees could be defined by extending the regular expressions by introducing an interleave (shuffle) operator. See reference [11] for more details.

In this thesis we will use the term regular grammar when we do not want to distinguish between ordered and unordered trees and hedges for ordered trees. Both tree definitions are used over an unranked alphabet, if not stated otherwise.

Example 3.3.1. Regular hedge grammar

```
G1 = (N1, T1, S1, P1),
N1 = {Milestone, MandatoryTask, OptionalTask, MandatoryData, Data}
T1 = {milestone, task, data}
S1 = {Milestone}
P1 = { Milestone→milestone (MandatoryTask OptionalTask*), MandatoryTask→task(MandatoryData), OptionalTask → task (Data), MandatoryData → mandatorydata (λ), Data → data (λ)}.
```

In Example 3.3.1 we show a grammar for milestone that contains tasks. The first task is mandatory, others are only optional.

Each grammar generates a language. We introduce here the formal definition from [10] for a regular tree language.

Definition 3.3.7. [10] An **interpretation** I of a tree t against a regular tree grammar G is a mapping from each node e in t to a non-terminal denoted I(e), such, that:

 $I(e_{root})$ is a start symbol where e_{root} is the root of t, and for each node e and its subordinates e_0 , e_1 , ..., e_i there exists a production rule $X \rightarrow a$ r such that

I(e) is X, the terminal (label) of e is a, and $I(e_0)I(e_1)...I(e_i)$ matches r.

Definition 3.3.8. A tree t is **generated** by a regular tree grammar G if there is an interpretation of t against G. [10]

Definition 3.3.9. A **regular tree language** is the set of trees generated by a regular tree grammar. [10]

3.3.1 Local tree grammars and languages

Local tree grammar is a restricted sub-class for a regular tree grammar. The interpretation is simplified, because each terminal (label) has associated one and only one non-terminal (there is no competition between non-terminals). This chapter is based on [10].

Definition 3.3.10. Let us have grammar G = (N, T, S, P). Let P1, P2 ϵ P such that

P1 has the form of $X \to a r_1$, P2 has the form of $Y \to a r_2$, where $X \neq Y$. Then we say the non-terminals X and Y **compete** with each other.

Example 3.3.2. Competing non-terminals

G2 = (N,T,S,P), where

N= {Database, Man, Woman, ManData, WomanData}

T = {database, person, manData, womanData}

S = { Database }

P = {Database → database (Man | Woman)*, Man → person (ManData), Woman → person (WomanData), ManData → manData (λ), WomanData → womanData (λ)}

In grammar G2 (Example 3.3.2), there are non-terminals Man and Woman that compete with each other.

Definition 3.3.11. **Local tree grammar** is a regular tree grammar without competing non-terminals. Language generated by a local tree grammar is a **local tree language**.

Example 3.3.3. Local tree grammar

```
G3 = (N, T, S, P), where

N= { Database, Person, ManData, WomanData}

T = { database ,person, manData, womanData}

S = { Database}

P = { Database → database (Person*), Person → person (ManData | WomanData), ManData → manData (λ), WomanData → womanData (λ)}
```

We have modified grammar G2 and merged the two non-terminals Man and Woman into a single non-terminal Person. Now Grammar G3 is a local tree grammar.

3.3.2 Single-Type tree grammars and languages

This subclass of regular tree languages is less restricted than local tree grammars.

- Definition 3.3.12. [10] A **single-type tree grammar** is a regular tree grammar such that
 - 1) for each production rule, non-terminals in its content model do not compete with each other, and
 - 2) start symbols do not compete with each other.

Language generated by a single-type tree grammar is a single-type tree language.

Example 3.3.4. Not a single-type tree grammar

Grammar G2 in Example 3.3.2 is not a single-type grammar. Again non-terminals Man and Woman in the production rule Database→database(Man|Woman)* compete.

Example 3.3.5. Single type tree grammar

Grammar G3 in Example 3.3.3 is a single-type grammar.

Example 3.3.6. Single-type tree grammar, not local tree grammar

G4 = (N, T, S, P), where

N = {Database, Men, Man, Women, Woman, ManData, WomanData}

T = {database, men, women, person, manData, womanData}

S = { Database }

P = {Database → database (Men Women), Men→men (Man*), Women→women (Woman*), Man → person (ManData), Woman → person (WomanData), ManData → manData (λ), WomanData → womanData (λ)}

Grammar G4 is a single-type tree grammar, but not a local tree grammar. Non-terminals Man and Woman compete, but they do not occur together in any content model.

3.3.3 Regular tree automata

Regular tree languages are recognized by finite regular tree automata. We introduce a definition of finite hedge regular tree automata here. This section is based on [11]. Some basic facts about automata can be found also in [10].

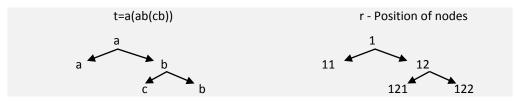
In previous section we have defined tree over ranked alphabet using ground term. For the definition of hedge automata below, we will redefine the tree using a bit different way. The following definitions are taken from [11].

Definition 3.3.13. A finite (ordered) **tree** t over \sum as partial function t: $N^* \rightarrow \sum$ with domain written **Pos**(t) satisfying following:

- 1. Pos(t) is finite, nonempty and prefix-closed,
- $2. \forall p \in Pos(t), \{j \mid pj \in Pos(t)\} = \{1..k\} \text{ for some } k \geq 0.$

Function Pos(t) returns all positions of nodes in a tree t. Position "pk" is the k-th child of a node at the position p. Generally an i-th child of a node x has the position defined as **iPos(x)**. Again we denote set of all trees over an alphabet Σ as $T(\Sigma)$.

Example 3.3.7. Tree and Pos()



In Example 3.3.7 we have tree t=a(ab(cb)) and a tree r from the same domain. The nodes of tree r are labeled by the Pos function. The value of t(11) is a – the first child of the root. The value of t(121) equals to c.

Now we define hedge automata.

```
Definition 3.3.14. [11] A nondeterministic finite hedge automaton (NFHA) over alphabet \Sigma is a tuple A = (Q, \Sigma, Q_f, P) where Q is a finite set of states, Q_f \subseteq Q is a set of final states, and P is a finite set of transition rules of the following form: a(R) \rightarrow q where R \in RegExp(Q), a \in \Sigma and q \in Q.
```

This definition defines bottom-up automata. That means that we process the leaves of a tree first and then we move up the tree towards the root.

Example 3.3.8. Example of NFHA

We want to define NFHA that accepts such trees that have a node c that contains somewhere in its descendants a node containing two children b. For example a tree t = c(ba(cbab)).

```
A1= (Q, \Sigma, Q_f, P), where Q = \{q, q1, q2, qf\} \Sigma = \{a,b,c\} Q_f = \{q_f\} Rules are: a(Q^*) \rightarrow q a(Q^* q1 Q^* q1 Q^*) \rightarrow q2 a(Q^* q2 Q^*) \rightarrow q2 a(Q^* qc Q^*) \rightarrow qc b(Q^*) \rightarrow q1 b(Q^* q1 Q^* q1 Q^*) \rightarrow q2 b(Q^* q2 Q^*) \rightarrow q2 b(Q^* qc Q^*) \rightarrow qc c(Q^*) \rightarrow q c(Q^* q1 Q^* q1 Q^*) \rightarrow q_f c(Q^* q2 Q^*) \rightarrow q_f c(Q^* qc Q^*) \rightarrow qc
```

In Example 3.3.8 we have defined NFHA with 12 rules. We mark nodes labeled by b with state q_1 . At the next layer, this state is transformed to state q_2 (if it contains at least two q_1) or back to default state q_2 . Please note the non-determinism here. Even if there are two children b of a node, there exists a rule that assigns a default state q_2 , but also a rule that assigns a state q_2 .

Next we define the **run** of the NFHA. For that we use the new definition of tree and the Pos() function.

Definition 3.3.15. [11] A **run** of NFHA $A=(Q, \sum, Q_f, P)$ on a tree $t \in T(\sum)$ is a tree $r \in T(Q)$ with the same domain as t such that for each node $p \in Pos(r)$ with a = t(p) and q = r(p) there is a transition rule $a(R) \rightarrow q$ of A with $r(p1)...r(pn) \in R$, where n denotes the number of successors of p.

Definition 3.3.16. [11] An unranked tree t is **accepted** by NFHA A if there is a run r of A on t whose root is labeled by a final state. The language L(A) of A is the set of all unranked trees accepted by A.

In Example 3.3.8 we have defined a NFHA A1. For a tree t = c(ba(cbab)) A1 assigns a set of states $s=\{q, q_1, q_f\}$. The tree t is accepted by A1 because there is a final state q_f in s.

We have defined nondeterministic bottom-up hedge automaton, let us define a deterministic one.

Definition 3.3.17. [11] A deterministic finite hedge automaton (DFHA) is a finite hedge automaton $A = (Q, \sum, Q_f, P)$ such that for all rules $a(R1) \rightarrow q1$ and $a(R2) \rightarrow q2$ either $R1 \cap R2 = \emptyset$ or q1 = q2.

The automaton A1 from Example 3.3.8 is not deterministic.

4 Taxonomy

In this chapter we compare the power of schema languages: DTD, XML Schema, Relax NG and Schematron. We assign each of them to a class of regular tree grammars. This chapter is based on [10] and [11].

4.1 DTD

Based on definition of DTD in [9], DTD requires a deterministic content model and more importantly contains the following restriction: "For Compatibility, it is an error if the content model allows an element to match more than one occurrence of an element type in the content model" [9]. Said in other words, an element - terminal – cannot have more than one corresponding non-terminal in an XML document. This is the definition of a local tree language.

4.2 XML Schema

We show that XML Schema corresponds to a single-type tree language. We present here the general idea. Proofs and examples can be found in [10] and [11].

One of the main features of XML Schema contrary DTD is the declaration and usage of types. XML Schema allows for elements with the same name to have different types and thus content model. Types allow XML Schema to overcome limitations of DTD (local tree language) and define for the same name of element different types of content.

The Usage of types is limited by a constraint called the "Element Declarations Consistent" [12]. This constraint says that all elements from the content model of an element that have the same name and namespace must also have the same type. E.g. there cannot be two book elements next to each other each having a different type.

The above constraint corresponds to the limitation of the single-type tree grammar and, thus, XML Schema belongs to the class of single-type tree languages.

4.3 Relax NG

We show the basic idea, that any regular tree grammar can be expressed in Relax NG. The construction of the schema can be found in [10] (However in [10] it is described for Relax Core and TRex, but modifying the process for Relax NG is straightforward).

Relax NG does not impose any restrictions for the content model. Its patterns (sequence, choice, one-or-more, zero-or-more) in the content model can be easily transformed to a regular expression. The pattern interleave can be also transformed to a regular expression. See the shuffle operator in [11].

4.4 Schematron

In previous chapters we classified DTD, XML Schema and Relax NG to their sub-class of regular tree language. To our best knowledge there is only little or no work that would classify Schematron to a sub-class of regular tree grammar. We found some recommendations and general algorithms for expressing schema models with Schematron in the blog of Rick Jelliffe [25].

In this thesis we introduce an algorithm for transformation of hedges into Schematron rules – Chapter 5. It this chapter we assign a sub-class of regular tree grammar to Schematron. We show that the expressive power of Schematron depends on the used query language.

Analysis

First we identify the differences of Schematron that concern the expressive power of validation and later we compare those.

The main difference between Schematron and other schema languages is the usage of rules. Classical grammar schema languages (like Schema or Relax NG) also use rules, but they do not name them like that. Grammar schema languages define types and elements. These definitions are in fact rules that validate the content. However, there is one big difference between the rules of Schematron and grammar schema languages – finding the context for the rule.

Identifying the context in grammar schema languages is trivial; we follow the structure of the document either from root to leaves or opposite. The previously processed elements identify the rule (or the set of rules) that should be used to validate current element. Note the previously identified elements create the context for the rules to come; that is the general idea of the validation algorithms. However, Schematron identifies the context for each rule independently. That means that the expressive power of Schematron is limited by the expression strength of the used query language.

The second aspect of validation is the validation of the content. From the formal definitions we know that the content for a regular grammar is expressed by a regular expression. So if the query language is able to express regular expressions, there should not be a problem.

We have shown that the expressive power depends on the expressive power of the query language – how well it can identify hedge. For the purpose of this thesis we will discuss the strength of XPath 1.0.

XPath 1.0 works only with the element names. So if we want to identify a path in a document, we have to translate types to their element names. This is one obstacle. The other one is that XPath 1.0 does not support regular expressions. In this thesis we use XPath 1.0 and we try to emulate the regular expressions. It can be done in the most cases but do not know if it is doable in all cases. This disadvantage could be removed by the use of XPath 2.0. However, there still persists the problem of context matching. In our analysis in Chapter 5 we discuss several ways how this could be done.

Even with the regex support, XPath is not able to identify all possible contexts. We can see that on the grammar G1 from Example 3.3.1. There are two types *MandatoryTask* and *OptionalTask*. Both use the label *task*, both are children of the same type. In the Example 3.3.1 the mandatory task is only the first child, but we could modify this grammar so it could be at any position. In that case XPath is not able to tell apart these two types.

We have shown a case where Schematron with XPath is not able to find context correctly. So there are two possible candidates for sub-class of regular tree grammar: local or single-type.

The context of local language is trivial, the names of element types are unique and XPath can handle these.

Lemma 2 Schematron with XPath with regex support is able to express singletype tree grammar.

The idea of proof is simple. We show the basic idea of construction of an XPath path for a single-type tree grammars.

Proof

Let us have a single-type grammar G with a starting type S.

We also know, that each child type of any type has unique label among its siblings.

For any type T, we create unique paths from starting type S to every occurrence of T in the grammar. Each step in a path uniquely identifies one of child types of the previous parent type. (Single-type grammar) ■

Summary

We have shown that the expressive power of Schematron mainly depends on the used query language. We have shown that if we are using XPath with regular expression support, Schematron is able to express single-type tree grammar.

5 Transforming hedges to Schematron schema

In this chapter we introduce algorithm for generating Schematron rules for a hedge. We use XPath 1.0 since it is widely spread, but we also suggest the possibility of using XPath 2.0.

We may encounter some limitations. As we will show, Schematron may not be ideal for expression general ordered unranked trees, since the schema for expressing that may be bigger than the schemas of classical grammar schema languages (e.g. Relax NG, DTD).

We divide the transformation process of a hedge into three steps. Step 1 will generate the correct context for rules that will be checked by steps 2 and 3. Step 2 controls the correct sum of children and step 3 matches the order of children to the regex of the hedge.

5.1 Definitions

Here we define terms that will be referenced in the following steps of the algorithm.

Let us have a hedge regular grammar G = (N, T, S, P) and a hedge $h: A \to a(R)$ where $h \in P, A \in N, a \in T$ and $R \in Regex(N)$.

Definition 5.1.1. We denote **production set S** to be the set of all nonterminals that occur in R.

Two examples of production sets are show below in Example 5.1.1.

Example 5.1.1. Example of a hedge h and S

```
h1: A \rightarrow a(B?C+)

S1 = \{B, C\}

h2: A \rightarrow a(BB?C*D*C)

S2 = \{B, C, D\}
```

Example 5.1.1 shows examples of hedges h1, h2 and their production sets S1 and S2.

Definition 5.1.2. We denote the translate function $trans: N \to T$ that assigns a terminal to a non-terminal.

Function trans is in fact a production rule without the regex part. Note that there can exist different hedges g, h that have the same terminal, i.e. trans(g) = trans(h).

5.2 Limitations

Before we describe the algorithm itself we introduce two limitations for the

algorithm that the grammar or the XML document must meet.

1) All sibling elements (sharing the same parent) with the same name must

be of the same type.

This constraint is similar to the "Element Declaration Consistent" [12] from XML

Schema. In other words if there is an element of type A, all its siblings with the same

name must have the same type A.

2) If there is a recursion within the derivation sequence of a non-terminal,

the recursion sub-sequence must be deterministic.

The second limitation is deeper explained in Chapter 5.3.5. This restriction is

needed because of the lack of regex support of XPath 1.0.

5.3 Step 1 - Context generation

The correct context for rules is absolutely necessary for the algorithm to work

correctly. The context is used to match an element in an XML document to a hedge

h from grammar G. The context is used for constraints generated by steps 2 and 3.

At first we show a trivial solution and discuss its disadvantages. Later we introduce a

more complex and reliable algorithm also including formal definitions and proofs of

correctness.

5.3.1 Trivial solution

The first thing that can come to a mind is the idea to generate context using relative

path and match only the element and maybe some of its ancestors.

Example 5.3.1. Trivial context matching

 $h1: A \rightarrow a(B?C+)$

XPath context: "//a"

50

In Example 5.3.1 we demonstrate a trivial way to match a context for a hedge. The hedge h1 is taken from Example 5.1.1.

This method may work if and only if there exists an inverse function $trans^{-1}$: $T \rightarrow \mathbb{N}$ to the function trans. In that case we can create a simple XPath expression for each hedge h using only relative path and the name of terminal of the hedge h.

Algorithm 5.3.1 Algorithm for trivial context

```
String TrivialContext(NonTerminal N) {
    string terminalSymbol = tran(N);
    return "//" + terminalSymbol;
}
```

In Algorithm 5.3.1 we have shown how to create a context from hedge. The result of this algorithm is show in Example 5.3.1 for hedge h1 from Example 5.1.1.

Summary

The trivial context generation may work, but with more strict condition than the limitation defined in Chapter 5.2. If we want to use relative context, there must not exist two different hedges with the same terminal. In other words, in the whole XML document, we must be able to identify a hedge based only on the name of the element. This satisfies only local tree grammars.

Example 5.3.2. Trivial context not working

```
h1: A \rightarrow a(B?C+)
XPath context: "//a"
h2: A \rightarrow a(BB?C*D*C)
XPath context: "//a"
```

Example 5.3.2 shows hedges from Example 5.1.1 and their generated trivial context. Both generated contexts are the same and thus the validation would not work correctly.

5.3.2 K-ancestors

This method is used for schema inferring in [27]. It is based on real data properties. Our trivial solution from Chapter 5.3.1 is, in fact, a specific case of this approach. In this chapter we will not describe the inferring method – it is described in Chapter 6.

The key idea is to identify context based on the element name and the name of K closest ancestors. For K = 2 it is the name of the element and the name of the parent. The trivial solution is a special case of this solution where K = 1.

Example 5.3.3. Example for K-ancestor solution

```
K = 2
G5 = (N, T, S, P), where
N= { Database, Person, Data}
T = { database ,person, data}
S = { Database}
P = { Database → database (Person*), Person → person (Data), Data → data(λ) }

XPath context for Person: "//database/person"
XPath context for Data: "//person/data"
```

Example 5.3.3 shows an XPath for identifying the context of the non-terminal Person and Data.

Algorithm 5.3.2 Algorithm for K-ancestors

```
String K_AncestorContext(NonTerminal N, int K) {
    var ancestors = get first K ancestors element names from N;
    string xpath = "/";
    foreach(var name in ancestors in reverse order) {
        xpath += "/" + name;
    }
    return xpath;
}
```

Summary

Similarly to trivial context generation, K-ancestor solution offers fast and comfortable way to identify context. On the other hand K-ancestor solution may not identify some context correctly -e.g. if we have K = 1 the situation is the same as for

trivial context. However, the real world data (described in [27]) show that more than 98% of context matching could be expressed with this solution and the K equal to 2 or 3.

5.3.3 Absolute path without a recursion

In the previous chapters we showed a trivial ways to identify a context and showed that these approaches are limited. In this chapter we introduce a more reliable, less restricted way to identify the correct context. We will use absolute paths to identify it.

This approach is sufficient for general cases of grammar that do not contain recursion in hedge transformation or only simple recursion.

Definition 5.3.1. We denote the **derivation sequence** D_A for non-terminal A to be a sequence of non-terminals produced by production rules that transformed the starting non-terminal to the non-terminal A of the hedge h.

Definition 5.3.2. We say that the derivation sequence D_A contains a **recursion** if there is at least one non-terminal $X \in D_A$ that occurs more than once in D_A . We say the recursion is a **simple recursion** if there are no other non-terminals between any two occurrences of $X \in D_A$.

Simple recursion is a sequence where the repetition of a single symbol is not interrupted by any other.

Multiple derivation sequences may exist for the same non-terminal. Without loss of generality, we suppose there exists only one such sequence. If more sequences exist, we can always merge their generated path expressions.

Definition 5.3.3. We denote **derivation sequence of terminals DT**_A for non-terminal A to be a sequence of terminals defined by the formula $\forall X \in D_A$: trans(X). Derivation sequence of terminals is a translated derivation sequence D_A .

The basic idea for generation of an absolute path is the following. When we want to find a context for hedge h, there exists a sequence DT_A of terminals. This sequence contains terminals that match an absolute path from the root element (that matches the terminal of the starting symbol) to an element a of the hedge h.

Example 5.3.4. Example of an absolute path without recursion

```
G6 = (N, T, S, P), where

N = { Database, Person, Data}

T = { database ,person, data}

S = { Database}

P = { Database → database (Person*), Person → person (Data), Data → data(λ) }

D<sub>Data</sub> = (Database, Person, Data),

DT<sub>Data</sub> = (database, person, data),

XPath<sub>Data</sub> = "/database/person/data"
```

Example 5.3.4 shows the derivation sequence for the non-terminal Data and the respective absolute XPath.

Algorithm for absolute path is trivial. We join the derivation sequence of terminals with "/". Please note that the derivation sequence is always deterministic. If there should be a non-deterministic step (e.g. operator "?" or "|") in derivation process from starting hedge to hedge h, we generate several deterministic sequences and merge all of their results.

5.3.4 Single recursion in production rules

In Example 5.3.4 we showed a simple example for absolute path context using only the child axis. However, there can be situations when the length of a derivation sequence (based on Definition 5.2) is not limited. This happens when there is a recursion in hedges. See Example 5.3.5. In this chapter we introduce algorithm for dealing with simple recursions that are special cases of recursions with deterministic content discussed in Chapter 5.3.5.

Example 5.3.5. Absolute path with simple recursion

```
G7 = (N, T, S, P), where

N= {Indent, Text}

T = {tab, text}

S = {Indent}

P = {Indent → tab (Indent | Text), Text → text(λ) }
```

```
DT<sub>Text</sub> = (tab, tab, ..., tab, text)

1) XPath<sub>Text</sub> = "//tab/text" <!—intuitive but not working -->

2) XPath<sub>Text</sub> = "//tab[count(ancestor::tab) = count(ancestor::*)]/text" <!-- working -->
```

Example 5.3.5 shows an example of a grammar with recursion in its production rules. There are presented two XPath expressions: 1) with only descendant-or-self axis and 2) with descendant-or-self axis and a condition checking the count of ancestors. Expression 1) will find any elements tab, including illegal sequences like (tab, tab, some-other-element, tab, text). Expression 2) locates only sequences that match the sequence DT_{text} .

We have introduced the problem and we extend Definition 5.3.1 to express recursion in derivation sequence.

Definition 5.3.4. We denote the **derivation regular expression DR**_A for non-terminal $A \in \mathbb{N}$ to be a word over Regex(N) that represents all derivation sequences of D_A .

 DR_A is able to express several derivation sequences with a single finite word. DRT_A is defined similarly.

Definition 5.3.5. We denote the **derivation regular expression for** $terminals \ DTR_A \ for \ non-terminal \ A \in N \ to \ be \ a \ word \ over \ Regex(T) regular \ expression \ over \ terminals \ T \ of \ grammar \ G. \ DRT_A \ is \ converted$ $from \ DR_A \ by \ the \ formula:$

$$\forall X \in DR_A \land X \in N: trans(X)$$

$$\forall X \in DR_A \land X \notin N: X.$$

We can re-define simple recursion using the derivation regular expression.

Definition 5.3.6. We say that derivation regular expression DR_A contains only **simple recursion** if and only if all regular operators + and * in DR_A are applied to a single symbol and not to a group.

Definition 5.3.7. Let us have a derivation regular expression DR and an xml fragment F. We denote **foreign elements** foreign(DR, F) to be such elements that have to be removed from F in order to be matched by the DR.

Since x+ can be expressed as xx*, without the loss of generality we can assume that all simple recursions consist of the form x*.

In Example 5.3.5 we can see path expressions for simple sequences. Now we introduce the algorithm for XPath generation for grammar with simple hedge recursion.

This algorithm creates XPath expression that matches undisturbed sequence (that may not be limited) of elements in the parent/child relation. Since we have only simple recursion and thus the repeating sequence consists of only single terminal, our work is fairly easy.

Since XPath 1.0 does not support regular expressions, we have to use the descendant-or-self axis with constraint on the ancestors. We create a constraint that will ensure that we will find only such descendants that have no element other than the element from the simple recursion.

The input is the DRT_A for the simple recursion. As denoted in this chapter, without the loss of generality the DRT_A will have the form of "x*".

The constraint is implemented using the count function, ancestor and descendant axes. The context for XPath evaluation must be taken at the start of recursion. Now the algorithm:

Algorithm 5.3.3 Context for simple recursion

```
/** Creates let statements under the PaternElement context and returns xPath expression that expresses the context

*/

string CreateSimpleContext(string DRTA, int iterationStartPosition, Context PaternElement) {

string subDRTA = DRTA.subSequence(0, iterationStartPosition);
```

```
string xPathContext;
    int recursionIndex = findSimpleRecursion(subDRTA);
    if (recursionIndex > -1) {
         //there is at least one simple recursion before the one we
want to analyze, e.g. "a* b x*"
         xPathContext = CreateSimpleContext(subDRTA,
recursionIndex, PaternElement);
    } else {
         //only absolute path, e.g. "a b c" => "a/b/c"
         xPathContext = CreateAbsoluteContext(subDRTA);
    }
    //create two let statements for variables that will be used in
generated xPath
    //variable for all ancestors
    string allCountVar = createUnitVariable("allCount");
    //form: <let name=" allCountVar" value="
count(xPathContext/ancestor::*)" />
    createLetVariable(allCountVar, xPathContext, "*");
    string iterationCharacter =
DRTA.getIterationCharacter(iterationPosition);
    //variable only for iterationCharacter occurences
    string charCountVar = createUnitVariable(iterationCharacter +
"Count");
    createLetVariable(charCountVar, xPathContext,
iterationCharacter);
    //return prefix//x[(count(ancestor::x) - $xCount) =
(count(ancestor::*) - $allCount)]
    return string.Format("{0}//{1}[(count(ancestor::{1}) - {2}) =
(count(ancestor::*) - {3})]", xPathContext, iterationCharacter,
charCountVar, allCountVar);
```

We summarize the above algorithm in short: We store into two variables counts of ancestors - any ancestor (allCount) and ancestors that are x (xCount). Since we

generate a Schematron schema we use the let construct for creating these variables. We generate the XPath expression for context: //x[(count(ancestor::x) - \$xCount)] = (count(ancestor::*) - \$allCount)]

Lemma 3 Algorithm 5.3.3 matches only the single recursion.

Let us prove that this algorithm does what it is supposed to. We use the absurdum proof.

Proof

Let us have a derivation sequence $(x_0, ... x_{i-1}, y_i, x_{i+1}, ... x_k)$ for some $i, k \in \mathbb{N}, 1 \le i \le k$. Let us assume that this sequence is matched with our algorithm. Without loss of generality we assume that the variables *allCount* and *xCount* are equal to 0.

Let us choose any $j \in \mathbb{N}$, $i < j \le k$. The element x_j follows y_i since i < j. From the sequence we can see that x_j has j preceding elements from which there are j-1 occurrences of element x. The constrain $count(ancestor::x_j) = count(ancestor::*)$ is thus false and XPath should not match the element x_j .

Note that the variables *allCount* and *xCount* allows us to ignore any sequence (any ancestors) before start of the simple recursion since they correct the equation correctly on both sides.

We have introduced the Algorithm 5.3.3 for simple recursion. See Example 5.3.6 for the result of this algorithm. The algorithm works also in cases when there are multiple simple recursions in serial order.

For cases when there is only absolute path before the simple recursion, the variables *xCount* and *allCount* are not necessary since the counts can be counted in generation time.

Example 5.3.6. Derivation sequence with prefix

```
DRT<sub>Text</sub> = book paragraph tab+ text

<schema xmlns="http://purl.oclc.org/dsdl/schematron" queryBinding="xpath">
...
<pattern></pattern>
```

Example 5.3.6 took the derivation regex DRT_{Text} from Example 5.3.5 and added a prefix to it. We show a fragment of generated Schematron schema with a single pattern containing two variables, tabCount and allCount, and an empty rule with context. Note that in this case we could omit the variables and could count the values directly from the sequence DRT_{Text} ; however, we leave it in the example to show the general approach.

5.3.5 Recursion with deterministic content

In the previous chapter we analyzed only derivation regular expressions with a simple recursion. In this chapter we introduce a general approach that allows us to match recursions with deterministic content.

In the first part of this chapter we analyze the situation. In the next part we introduce and describe limitations and in the last part we propose an algorithm for Schematron context generation.

We denote the **derivation loop** to be a part of a derivation regex that is being repeated. (The inner part of the recursion.)

Analyses

We use the formalism defined for simple recursion and enhance it for a more general situation.

```
Example 5.3.7. DR_A and DRT_A
G7 = (N, T, S, P), \text{ where}
N = \{S, A, B, C\}
T = \{a\}
```

```
S = \{S\}
P = \{S \rightarrow a \text{ A, } A \rightarrow a \text{ } (B \mid C \mid \lambda), B \rightarrow a \text{ } (A), C \rightarrow a \text{ } (A) \}
DR_A = S(AB?) + (AC?)* \text{ or } DR_A = S(A(B \mid C)) + DRT_A = a(a(a \mid a)) +
```

In Example 5.3.7 we show the DR_A can have more than one expression and that the according DRT_A can look totally different.

Definition 5.3.8. We denote the **lead terminal** of the recursion DR_A to be the first terminal of DRT_A .

The lead terminal is the first terminal that is repeated. This terminal is interesting for us, because it starts a new sequence in recursion and, if we can identify it, we can identify the whole sequence.

Example 5.3.7 showed us that identifying the lead terminal may not be so easy. In the following text we introduce some limitations that will help us in identification of lead terminals.

Limitation

The general situation is much trickier than the one of simple recursion. There can exist nested recursions. In fact, we would have to rewrite general regular expression for children and descendants into XPath 1.0. That is very problematic and even may not be solvable. The introduced limitation in this chapter will ensure that our algorithm will work, if the task satisfies this limitation.

The content of the recursion must be deterministic.

We do not allow for any of these symbols: ? * + |

Now we show some examples that show the problem of non-deterministic content. As we will see in the description of our algorithm, we use similar constructs as in the algorithm for simple recursion – counting the ancestors from descendants. Any non-determinism within the recursion could lead into false match. See simplified Example 5.3.8.

Example 5.3.8. False match in context

```
DRT<sub>A</sub> = (abb+)*

Context regex = //a[count(ancestor::a) <= (2*count(ancestor::b))]

False match: a/b/b/b/a/b/a
```

Example 5.3.8 shows an example of false match of context. The XPath for context matches the first and the last element a. But it should match only the first one. The reason for matching the last element a is that the count of elements b from the first cycle of recursion (3) plus the count from the second cycle of recursion (1) gives up 4 b-ancestors. This satisfies the constraint for the last element a.

The limitation ensures that the number of elements in recursion are deterministic and our algorithm will be able to match the correct context.

Algorithm for deterministic loop

In this chapter we describe the algorithm for general context generation. We will extend the algorithm introduced for simple recursion - Algorithm 5.3.3. There we used descendant-or-self axis with constraint to a single element and checked that there are no other elements in the axis. We will use this construct, but for our needs we will extend it and add several more constructs and constraints.

The constraints that will our algorithm check are:

- **Lead terminal** constraint
- **Restriction** no foreign elements are present in a matched sequence
- Completeness constraint matching the elements to derivation terminal regex.

The **lead terminal** constraint ensures that we match the correct lead element. This constraint may not be used every time, but it is important to notice a situation when there could be multiple elements of the lead symbol. We refer to Example 5.3.7.

In the algorithm for simple recursion - Algorithm 5.3.3 – we used only the **restriction** constraint. Since now there can be more than just one element within recursion loop, we are going to slightly improve this constraint.

The restriction constraints checks only that there are no foreign elements; the **completeness** constraint checks that all terminals from derivation terminal regex are matched to elements within the recursion, thus no elements are missing and all elements are in correct order. This will ensure that we ignore all other permutated sequences.

The algorithm will match all possible lead terminals in the descendant axis and identify the correct ones. We have to ignore all other terminals that are neither a part of the recursion, nor the lead terminal (e.g. another terminal with the same name as the lead terminal but occurring inside the recursion loop at a different position). We will describe the algorithm in three parts — each for a constraints described above. Each part will produce a predicate for XPath.

To identify the lead terminal we count the ancestor elements that match the lead terminal and modulo the value. Part I can be omitted if the lead terminal occurs only once within the recursion loop.

Algorithm 5.3.4 Algorithm for recursion Part I – Modal Count

```
string GetModuloConstraint (DRT terminalRegex, Context PaternElement) {
    string LeadTerminal = getLeadingTerminal(terminalRegex);
    int moduloCount = terminalCountInRecursion(terminalRegex, LeadTerminal);

//variable lead terminal occurences
    string leadTerVar = createUnitVariable("modulo" + LeadTerminal);

//form: < let name="leadTerVar" value="count(ancestor::x)" />
    createLetVariable(leadTerVar, xPathContext, iterationCharacter);

//return (count(ancestor:: x) - $modulo_x) mod x0 or return string.Format("(count(ancestor::{0}) - {1}) mod {2} = 0", LeadTerminal, leadTerVar, ModuloCount);
```

}

Lemma 4 Algorithm 5.3.4 finds the correct lead terminals.

Proof

Since we do not allow any nondeterministic behavior within the recursion loop, the number of terminals that have the same name as the lead terminal is fixed. ■

Example 5.3.9. Example for algorithm for recursion part I - The lead terminal

```
DRTA = (aa)*

Generated predicate:

P1 = count(ancestor::a) mod 2 = 0

Context:

//a[P1]
```

Example 5.3.9 shows a predicate for matching the lead terminal a.

Algorithm 5.3.5 is based on Algorithm 5.3.3 for simple recursion. The Algorithm 5.3.3 was used only for simple recursion, and, thus it checks only a single element. We enhance it to support checking of multiple elements. The description is brief; please look at the algorithm for simple recursion first.

Algorithm 5.3.5 Algorithm for recursion Part II - restriction

```
string CreateRestrictionContext(string DRTA, string xPathContext, Context PaternElement) {

//we create n + 1 variables, where n is the number of distinc terminals in DRTA

string allCountVar = createUnitVariable("allCount");

//form: <let name=" allCountVar" value=" count(xPathContext/ancestor::*)" />

createLetVariable(allCountVar, xPathContext, "*");

string result = "";

foreach (var terminalCharacter in distinct terminals of DRTA) {

string charCountVar = createUnitVariable(terminalCharacter + "Count");

createLetVariable(charCountVar, xPathContext, terminalCharacter);
```

The proof of correctness is very similar to that presented for Algorithm 5.3.3.

Example 5.3.10. Example for algorithm Path II - Restriction

```
DRT<sub>A</sub> = (abcb)*

Generated predicate:

P2 = (count(ancestor::a) + count(ancestor::b) + count(ancestor::c)) = count(ancestor::*)

Context:

//a[P2]
```

Example 5.3.10 shows a generated predicate for restriction constraint. For simplicity we do not use variables since the DRT_A has no prefix before the recursion.

The following part of our algorithm generates the **completeness** constraint about the internal structure of the recursion loop.

The aim of Algorithm 5.3.6 is to check that the internal structure of the recursion loop matches the regular expression of DRT_A. The generated conditions by this part of the algorithm will ensure that the loop contains all necessary elements and that they are in a correct order. Since the loop itself is deterministic, the problem ahead is simplified.

To check the internal structure of a recursion loop, we use nested child condition. In a single condition we check the child, grandchild, great-grandchild... of the lead terminal. We denote this condition as the structural check.

The generated constrain will check the count of ancestor lead terminals against the count elements found by the structural check.

We transform the deterministic loop into the structural check:

```
leading_symbol[child[grand-child[...[leading_symbol]]]
```

The final parent-child check is matching the lead symbol of the following recursion loop.

We count the number of occurrences of the lead terminal in the loop. We will internally denote this constant as \$LeadingSymbolCount.

Thanks to the facts that the loop is deterministic, we can afford to check the internal structure by a single nested XPath condition. We have transformed the loop e.g. "abcad" into the XPath a[b[c[a[d[a]]]]]. The generated condition will be the following:

```
count(ancestor::a) = $LeadingSymbolCount * count(ancestor::a[b[c[a[d[a]]]]])
```

The DRT_A for the loop is *abcad*, the lead symbol is thus a and the constant \$LeadingSymbolCount\$ expresses the number of symbols of the lead terminal within the recursion loop. Here it is equal to two.

Algorithm 5.3.6 Algorithm for recursion Part III – minimal validity and order

```
String generateStructuralCheck(string DRTA) {
    string terminal = getLastTerminal(DRTA);
    string prefix = getPrefixWithoutLastTerminal(DRTA);
    if (prefix == "") {
        return terminal;
    } else {
        return string.format("{0}[{1}]", terminal,
        generateStructuralCheck(prefix));
    }
}
/** parameter DRTA contains only the body of recursion, not a prefix
```

```
*/
String getCompletenessConstraint(string DRTA) {
    string leadTerminal = getFirstTerminal(DRTA);
    int LeadingSymbolCount = count(leadTerminal, DRTA);
    string structuralCheck = generateStructuralCheck(DRTA + leadTerminal);
    return string.format("count(ancestor::{0}) = {1} * count({2})", leadTerminal, LeadingSymbolCount, structuralCheck);
}
```

Lemma 5 Algorithm 5.3.6 identifies only the lead terminals preceded by a complete deterministic recursion body and the recursion body is in the correct order.

Proof

The structural check ensures that the matched lead terminal is followed by elements in the correct order and none is missing.

The final part of the structural check – the condition that checks the lead terminal of the next recursion loop - ensures that structural check checks the whole structure of the loop. (Not only a part of it). ■

The algorithm for more general recursions consists of three parts. Each part focuses on a different problem. All together it ensures that the recursion with a deterministic loop can be identified.

Summary

We have shown the algorithm for more general cases. However, we do not allow non-deterministic content in the recursion loop, because XPath 1.0 has only very limited support for regular expression matching.

Algorithm 5.3.6 could be improved to allow some non-deterministic content. The way to do so is to split the single XPath sequence into more parts and for each non-determinism check all possible children/sub-sequences. The main obstacle is that there could accumulate some sub-sequences in the previous loops and these sub-

sequences could falsely satisfy the condition for loops that have these subsequences missing – see Example 5.3.8.

5.3.6 Context for each hedge of grammar

We have introduced several algorithms, i.e. several ways to create the context for a hedge in the grammar G. In this chapter we identify cases where each of the algorithms should be applied.

Let us have a grammar G = (N, T, S, P) and a set of hedges. We create a directed graph $\vec{G} = (V, E)$, where V is a set of vertices and V = N, E is a set of edges and $E = \{XY | X \to xR \in P \land Y \in R\}$. Edges of the graph express the derivation process of the grammar.

The idea of Algorithm 5.3.7 is as follows. We have the starting set of non-terminals from the grammar. This starting set can be extended at the beginning by non-completing non-terminals. We use the BFS (breadth-first search) algorithm from the starting set of non-terminals to process all non-terminals/vertices. We use BFS so that we can utilize the already generated context of preceding vertices.

Algorithm 5.3.7 Context for grammar

```
void CreateContext(grammar G) {
    DGraph = createDirectedGraphFromGrammar(G);
    foreach(var start in G.S) {
        BFS(start, G);
    }
}

void BFS (vertex Start, grammar G) {
    fifo f = new fifo();
    fifo.push(Start);

while (not fifo.empty()) {
        vertex V = lifo.pop();
    }
```

```
if (V.visited) {
           continue;
     }
     If (isNotCompeting(V, G)) {
           generateTrivialContext(V, G);
     } else {
          var DRA = generateDRA(V);
          if (isRecursionFree(DRA)) {
                generateAbsoluteContext(V, G);
          } else if (containsSimpleRecursion(DRA) {
                generateSimpleContext(V,G);
          } else {
                //we suppose the recursion is deterministic
                generateGeneralContext(V,G);
          }
     }
     V.visited = true:
     Foreach(var follower in V.followers) {
          fifo.push(follower);
     }
}
```

We can utilize variables of Schematron and store the contexts for all non-terminals that correspond to lead terminals. The use of trivial context generation is optional, the algorithm will work without it.

Please note that this step only identifies context. The validation is done in steps 2 and 3.

5.4 Step 2 - Boundary rules

In Step 1 we identified context for rules that will be generated by the second step and by the following third step. The found context will be denoted as CONTEXT. In this step we focus on a simple validation using minimum and maximum occurrence checks – boundary rules – of elements from the regex part R of the hedge h. We can detect elements that are not present in the regex R and elements with invalid occurrence.

We process the regex R and for each non-terminal X from production set S (Definition 5.1.1) we count the minOccurs and maxOccurs based on Algorithm 5.4.1. Both functions are defined as follows: minOccurs: $N \to \{0,1,2,...\} \cup \{unbounded\}$, maxOccurs: $N \to \{0,1,2,...\} \cup \{unbounded\}$, where N is the set of non-terminals.

Algorithm 5.4.1 Algorithm for counting minOccurs and maxOccurs

```
number minOccurs(n, regex) {
    If (regex.length <= 1) {
         return regex == n ? 1 : 0;
    var operator = getOperator(regex);
    var r1 = getFirstOperand(regex), r2 = getSecondOperand(regex);
//r2 can be empty
    switch(operator) {
    case sequence:
         return minOccurs(n, r1) + minOccurs(n,r2);
    case choice:
         return min(minOccurs(n, r1), minOccurs(n,r2)); //use max()
for maxOccur
    case optional:
         return 0; //return maxOccurs(n, r1) for maxOccurs
    case plus:
         return minOccurs(n, r1); //return unbounded for maxOccurs
    case asterix:
```

```
return 0: //return unbounded for maxOccurs

case group:

return minOccurs(n,r1);
}
```

In Algorithm 5.4.1 we use a pseudo-code and recursively parse the regular expression until we get to a single non-terminal. Based on regex operator used, we process the result of the inner regular expression. Note that we count with unsinged integers and the special value 'unbounded'. Any add operation with this special value return again the value 'unbounded'.

The function maxOccurs is very similar and the differences are stated in the code of function minOccurs.

Example 5.3.11. Example of minOccurs and maxOccurs

```
minOccurs(B, B?C+) = 0 \qquad minOccurs(C, B?C+) = 1 maxOccurs(B, B?C+) = 1 \qquad maxOccurs(C, B?C+) = unbounded minOccurs(B, BB?C*D*C) = 1 \qquad minOccurs(C, BB?C*D*C) = 1 maxOccurs(B, BB?C*D*C) = 2 \qquad maxOccurs(C, BB?C*D*C) = unbounded
```

In Example 5.3.11 we show on regular expression from Example 5.1.1 the values returned by function minOccurs and maxOccurs.

We abbreviate the function calls of minOccurs and maxOccurs by allowing leaving out the second parameter. The default value is the regex *R* of hedge *h*.

Now we get to the rule generation. With defined function *minOccurs* and *maxOccurs* we can generate rules for hedge *h*. We use the function of XPath *count*. First we check that there are no illegal children with a single rule:

$$\sum_{s \in S} count(trans(s)) = count(\text{child} ::*)$$

Where child::* is an XPath expression for any child element from current context.

Next, we generate a rule for each non-terminal from S to check the bounds (minimum occurrence and maximum occurrence):

$$\bigvee_{s \in S} \{count(trans(s)) \ge min0ccurs(s) \land count(trans(s)) \le max0ccurs(s)\}$$

Note that we may skip the maximum bound check, if maxOccurs equals to the value 'unbounded'. The same fact can be applied to minOccurs and the value 0.

Example 5.3.12. Boundary rules for hedge h1

Example 5.3.12 contains generated Schematron rules for hedge h1 from Example 5.1.1. We assume that trans(B) = b and trans(C) = c.

5.5 Step 3 – order checks

In step 2 we generate constraints for boundary counts of elements. For unordered unranked trees these rules would be sufficient. However, we are generating rules for ordered unranked trees and that is why we need Step 3.

XPath 1.0 does not support regular expressions, the only thing we can do is to construct several rules that use XPath-axes (preceding, following, etc.) and try to express the regular expression with it. The full expression of a hedge using Schematron rules can be found in Chapter 2.2. The basic idea is taken from [25].

We recapitulate in short what we want to do. We have a hedge h with a regular expression R for its content. We want to generate rules that check that the content (the child elements) match the regular expression.

5.5.1 Basic idea of the algorithm

We have a regular expression *R* and element e. We want to create a set of rules for Schematron to test the order of child elements of e. We process the regex R sequentially from left to right. For each part of the regex we create constraints for allowed following siblings. A more complex regular expression may require more rules to express it.

Generally we mimic the work of an NFA. We determine the state we are in and thus we know what transitions are allowed. If we detect any other following sibling we report it.

The names of XPath axes are long, so we denote several abbreviations:

- Fn = following-sibling::*[1][self::n] //the first sibling on the right is n
- Pn = preceding-sibling::*[1][self::n] //the first sibling on the left is n
- Dn = preceding-sibling::n //there is some preceding sibling (on the left)
 which is called n

We can concatenate these abbreviations:

• PaPb = preceding-sibling::*[1][self::b][preceding-sibling::*[1][self::a]] or with an equivalent

preceding-sibling::*[1][self::b] and preceding-sibling::*[2][self::a]

PaDb = preceding-sibling::b[preceding-sibling::*[1][self::a]]

Regular expression operators, except the grouping operator, can be expressed using conditions on following siblings - see Example 5.5.1. Based on the cardinality of the following (or preceding) siblings, we may use more than just one condition (see Example 5.5.2).

Example 5.5.1. Transformation of a sequential regex

In Example 5.5.1 we expressed a simple regex that contains only a sequence of three elements -x, y and z. We created three rules with help of abbreviation defined at the beginning of step 2. Each rule checks the follower to match the following element from regex. We also added border conditions for elements at the beginning and end of the regex.

Example 5.5.2. Transformation of a regex with a non-trivial cardinality

Example 5.5.2 extends Example 5.5.1. We have added a non-trivial cardinality for elements x and z. The regex allows a sequence of elements x at the beginning and makes the element z optional. The first and second rules must be extended to capture the new conditions — element x must be the first element or be preceded by another element x and must be followed by x or y. Element y must be followed by an element z, or be the last element. Only the last (third) rule remains the same, because the element z (if present) can be only the last element.

In Example 5.5.1, Example 5.4 and Example 5.5.2 we demonstrated the idea of generating rules for regular expression. Now we describe the problem in more detail.

5.5.2 Problem analysis

The Schematron rules are independent of each other and thus make sequential processing of a regex more complicated. The main problem is to match an element to a part of a regex. If we succeed in identifying the correct position in the regex, the testing of the following sibling is fairly easy.

Elements with multiple occurrences in the regex represent the main problem - see Example 5.5.3. We have to distinguish them using only XPath 1.0.

Example 5.5.3. Double occurrence of an element in a regex

```
R = a?a?
L(R) = {\lambda, a, aa}
```

In Example 5.5.3 we can see a regex that contains two occurrences of a, each one is optional. The word "a" generated by the regex R is generated by either the first or the second element a.

In order to simplify the work with this task, we transform the regex to NFA [26]. Each state in the NFA can have multiple paths (words) to access it (or produce the state). In Example 5.5.3 the first element a is produced only by the empty word λ and the second element a is produced by words λ and a. Note that both elements a are produced by the empty word λ , but only the second one is produced also by a word a. This illustrates the general problem — each state is produced by a set of words, different states can have non-empty intersection of these sets.

Definition 5.5.1. Let us have a NFA =
$$(Q, X, \delta, q, F)$$
. We denote the **production set** of the state $p \in Q$ as **Product** $(p) = \{w \in X^* | \delta^*(q, w) = p\}$.

Using this definition we can write the production sets for states for regex in Example 5.5.3 as Product(a1) = $\{\lambda\}$ and Product(a2) = $\{\lambda, a\}$.

Let us have two states p and q that have a non-empty intersection P of their production sets. When we receive a word from P, the active state of the NFA can be either p or q. This means that the next allowed state can be the follower of either state p or q.

The solution for our problem with multiple elements in a regex is the following. When we have an element x that is present in the regex R more than once, we compute the production sets for each occurrence of x and intersect them. We merge the rules for words that are in some intersection, since they are not differentiable.

5.5.3 Algorithm

We have a regex R and want to create Schematron rules for validation. We analyzed the problem in the previous chapter. Now we introduce our algorithm for transforming the regex into Schematron rules.

Algorithm 5.5.1 Transformation of regular expression to Schematron rules

```
void generateRules (regex R, context C) {
   var terminals = getTerminalSet(R);
   foreach(var terminal in terminals) {
      if (count(terminal, R) == 1) {
           generateSimpleRule(terminal, R, C);
      } else {
           generateComplexRule(terminal, R, C);
      }
   }
}

void generateSimpleRule (string T, regex R, context C) {
   var element = getElement(T, R); //find the corresponding element for terminal in R
   var followers = getFollowers(element, R);
```

```
writeRule(T, null, followers); //there are no conditions for this
terminal
}

void generateComplexRule (string T, regex R, context C) {
    var paths = getPaths(T, R); //find all paths that lead from states of
terminal T to the start of Regex.

    var prefixAutomaton = PrefixAutomaton.EMPTY;
    foreach(var path in paths) {
        mergeNFA(prefixAutomaton, path);
    }

    foreach(var terminalState in prefixAutomaton.outputs) {
        var condition = getCondition(terminalState);
        var followers = getFollowers(terminalState, mergedNFA);
        writeRule(T, condition, followers);
    }
}
```

Let us describe Algorithm 5.5.1. We generate rules for each terminal in the regular expression. If the terminal has only a single occurrence in the regex, we generate a single rule without any complex conditions. Otherwise we have to tell apart each occurrence of this terminal in the regex since the followers may differ.

In method generateComplexRule we find a list of all words that lead to the terminal (see the production set from Definition 5.5.1). Multiple words can lead to the same terminal. To find all the words we can use a NFA with reverted production function and keep the found words represented as an automaton. We will merge those automatons into a single prefix automaton. This automaton will serve as the source for conditions to tell apart terminals T at different positions in the given regex R.

In the above paragraph and also in Algorithm 5.5.2 we use the term prefix automaton. It is an extended NFA that contains one additional symbols in the input alphabet - $^{\circ}$. Symbol $^{\circ}$ means the same as in the common regex usage - no

preceding symbol. In the prefix automaton we have two categories of states – whether they have a transition to a following state (**node** state) or not (**leaf** state).

Algorithm 5.5.2 Merging NFA of terminals

```
void mergeNFA(prefixA aut, NFA nfa) {
    var mapping = initMapping();
    var mapped = mapping[nfa.startingState];
    if (mapped != null && mapped != aut.start) {
         update mapping with mergeAutomatonStates(aut.start,
mapped);
   } else {
         Add new mapping for nfa.startingState and aut.start
    doMerge(nfa.startingState);
void doMerge (NFAState startingState) {
    var mapping = initMapping();
    var lifo = LIFO.emptyLifo;
    lifo.push(startingState);
    while (not lifo.isEmpty()) {
         var state = lifo.pop();
         var automatonState = mapping[state];
         switch(automatonState.type) {
         case NODE:
               foreach(var trans in state.forwardTransitions) {
                    if (automatonState.hasTransition(trans.letter) {
                         handleExistingTransition(automatonState,
lifo, trans);
                    } else {
                         createNewTransition(automatonState, lifo,
trans);
```

```
}
              }
              break;
         case LEAF:
              if (automatonState.nfaReference.isEmpty()) {
                    automatonState.nfaReference.add(state);
              } else if (isDifferentNFA
(automatonState.nfaReference[0], state)) {
                    // the same prefix part, we need to update this
state
                    lifo.push(state); //repeat the evaluation for this
state, after this leaf is processed (either changed to NODE or
FINAL_LEAF);
                    var leafState = automatonState.nfaReference[0];
                    if (leafState.forwardTransitions.length > 0) {
                         automatonState.type = NODE;
                         lifo.push(leafState);
                    } else {
                         automatonState.type = FINAL LEAF;
                    }
              }
              break:
         case FINAL LEAF:
              automatonState.nfaReference.add(state);
              break;
   }
void createNewTransition (AState automatonState, LIFO lifo,
Transition trans) {
    if (mapping.contains(trans.finalState)) {
```

```
automatonState.connectToState(mapping[trans.finalState]);
    } else {
         var createdState =
automatonState.createTransitionState(trans.letter);
         //asociate the newly created automaton state with the NFA
state
         addMapping(trans.finalState, createdState);
    }
    lifo.push(trans.finalState);
}
void handleExistingTransition (AState automatonState, LIFO lifo,
Transition trans) {
    var foundAState = automatonState.forwardTransitions[trans.letter];
    if (no mapping for trans.finalState) {
         //this state in NFA is was not yet visited, associate it with this
automaton state
         trans.finalState.image = foundAState;
         addMapping(trans.finalState, foundAState);
         lifo.push(trans.finalState);
    } else if (trans.finalState.image != foundAState) {
         //state from NFA cannot point to two different automaton
states -> merge them
         var mergedAState =
mergeAutomatonStates(trans.finalState.image, foundAState);
         updateMapping(trans.finalState, mergedAState);
         lifo.push(trans.finalState);
    } else {
         //already visited
    }
```

```
AState mergeAutomatonStates(AState state1, AState state2) {
    //state LEAF may change to NODE or FINAL LEAF, we need to
be certain of the outcome
    If (state1.type == LEAF) {
         doMerge(state1.nfaReference[0]);
    }
    If (state2.type == LEAF) {
         doMerge(state2.nfaReference[0]);
    }
    //now we have only type NODE or FINAL LEAF
    If (state1.type == FINAL LEAF || state2.type == FINAL LEAF) {
         //merge into single FINAL_LEAF, destroy possible following
states in the automaton
         state1.type = FINAL LEAF;
         state1.nfaReference.add(state2.nfaReference);
         state1.removeTransitions():
         state1.replaceState(state2);
    } else {
         //both states are of type NODE, merge their followers
recursivly
         state1.nfaReference.add(state2.nfaReference);
         state1.replaceState(state2);
         foreach (var trans in state1.forwardTransitions) {
              if (state2.hasTransition(trans.letter) {
                    trans.finalState =
mergeAutomatonStates(trans.finalState, state2.transition[trans.letter]);
//recursive merge
                    state2.removeTransition(trans.letter);
              }
         //add the rest of the transition from state 2
         state1.forwardTransitions.add(state2.forwardTransitions);
```

```
}
return state1;
}
```

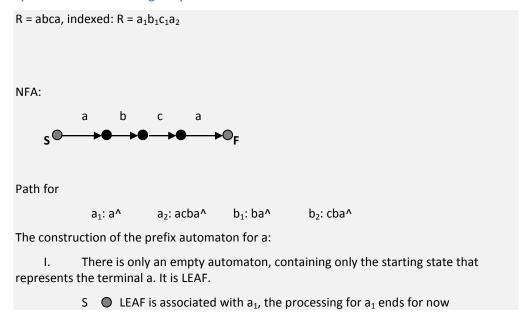
In Algorithm 5.5.2 we introduce the algorithm to create a prefix automaton. The prefix is constructed from the position of the terminal in regex R in the direction to the beginning of the regex R. We want to find unique suffixes of prefixes or to know that some prefixes cannot be decided.

In our prefix automaton the leaf states will contain a reference to NFA of terminals and their follower list. Any leaf state identifies a word that identifies a specific terminal.

This algorithm starts in the state that represents the terminal in the NFA and the starting state of the prefix automaton. We simulate all the paths from the NFA in the prefix automaton and add new states to it. We connect states from processed NFA to the states of the automaton – to detect cycles. Each state from NFA can have at most one connection to a state in the automaton.

Now we can build the prefix automaton. Example 5.5.4 shows a process of building the automaton step by step.

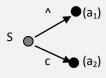
Example 5.5.4. Building the prefix automaton



- II. Processing a2. The starting state is also a LEAF for a1. The NFA (path) for a_1 contains another symbol: $^{\land}$. We change the type of the starting state to NODE. And process a_1 further.
- III. We create a new state for a_1 LEAF for symbol ^. The processing for a_1 ends here.



IV. We continue processing of a_2 . We create a new state (LEAF) for symbol b and end. We do not need to continue, since we found unique suffixes of prefixes for both a_1 and a_2 .



Example 5.5.4 show the work of Algorithm 5.5.2 – the creation of a prefix automaton for terminal a.

Conditions generation

After creation of the prefix automaton we can start to generate rules. From the prefix automaton we know what states are easily distinguishable and what states are similar (share the same output state). We do use the word similar, because if there exists a cycle on a path from automaton start to the output state, there can also exist a hidden condition for the repetition counts. Each of the similar states can have a different repetition condition. See Example 5.5.5.

Example 5.5.5. Example of similar states in prefix automaton

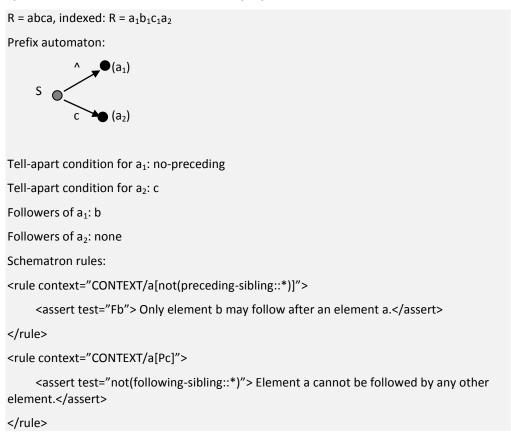


Example 5.5.5 shows that even a distinct occurrence of a terminal in a regex can be merge into a single state in the prefix automaton. We must not express this

situation by only a single rule (as it may look correct at first sight) since symbol "c" can only occur after even number of symbols "a".

If there is no cycle in the path, we can generate the Schematron rule for that terminal of the output state. See Example 5.5.6.

Example 5.5.6. Schematron rules for simple prefix automaton



Example 5.5.6 shows the generation of rules and conditions from prefix automaton created in Example 5.5.4.

Cycle handling

Example 5.5.5 showed us that our algorithm is not perfect. However, we will not show a solution for this problem in this thesis and leave it for a future work.

Future optimizations

There are several aspects that can be done to improve the performance of generated rules. This chapter is merely for motivation purposes for future work.

As we saw in Example 5.5.5 it can happen that more occurrences merge in the prefix automaton, leaving only a single rule and thus does not need additional condition like other complex rules.

Another feature of our algorithm is that for each output state of the prefix automaton there is generated a rule with a single Schematron assert. Again this could be improved by merging similar rules and adjusting asserts.

Another possible optimization would be the use of XPath 2.0. XPath 2.0 supports regexes that would help greatly in Schematron schema generation. However, using a simple regex for validating content has a downside –asserts are simplified and will not tell the user where exactly an error is.

5.6 Summary

We have shown that expressing hedges with XPath1.0 is possible, but contains some limitations. In this chapter we summarize these limitations and identify the sub-class of regular grammar that we can express.

We introduced three-step algorithm. Step 1 generates correct context for later steps. Steps 2 and 3 generate Schematron rules. All steps introduce a limitation for the content — we are unable to differentiate types. Thus we cannot allow two different types for a single element in the same content model, i.e. we do not allow competition between non-terminals. This restricts the grammar to a Single Type tree grammar.

Step 1 introduces another limitation. It does not allow for any non-determinism in the recursion of the grammar. This is limited neither by a local tree grammar, nor by a Single type grammar. However, as we will see in the next chapter, the k-ancestor approach offers a nice way to handle the most real-world data.

Step 3 matches regular expression of a hedge. We have shown an approach that uses XPath 1.0. We also showed that there are some cases where our algorithm may not work – i.e. tell apart odd and even number of preceding siblings. Step 3 can be omitted if we want to generate rules for unordered hedges.

The expression strength of our algorithm is thus limited by step 1 and 3. In may be possible to improve the algorithm from step 3 and utilize it also for step 1 and lift some limitations, but that is a possible task for a future work.

6 XML Schema inferring

This chapter describes ways of XML schema inferring. We will not go into deep details, because this problem has been analyzed many times before, but we will describe single method more deeply since we use it in our implementation. A deeper analysis can be found for example in [28] and [29].

There are two different general approaches to XML schema inferring – heuristic approach and grammar-inferring approach.

Heuristic approaches come from practical needs. They utilize empiric observations and are more human-oriented. Results of heuristic approach are created by generalization of a simple schema based on empiric observations (e.g. if an element occurs three or more times, we denote it as unbounded). Based on this fact, the inferred schemas cannot be assigned to a specific type of grammar.

Grammar-inferring approaches are based on a theoretical basis. Each method of this family generates defined grammar type. However, based on the Gold's theorem [31], the language cannot be learned only from positive examples. As such, there has to be typically some user input to direct the algorithm to the result.

6.1 iXSD

This algorithm was introduced in [30]. It is a grammar-inferring approach that generates single-type grammar (in the form of XML Schema - XSD).

The authors of this method analyzed the real world data and came with two following observations:

- Locality [30]: The content model of an element in more than 98% of XSDs in practice turns out not to depend on the whole labeled path from the root to the element, but only on the k last element names in that path, with typically $k \leq 3$.
- **Single occurrence** [30]: The regular expressions in more than 99% of XSDs in practice are of a very specific form: *each element name occurs at most once in them.*

We use these observations in the following definitions.

- Definition 6.1.1. We denote an XML document **k-local** if any of its content models depends at most on the last **k** labels of ancestors.
- Definition 6.1.2. We denote **single occurrence regular expression** (**SORE**) to be a regular expression $R \in Regex(L)$, where each symbol $l \in L$ is present at most once.

```
Example 6.1.1. SORE
S_1 = a+b?c \text{ is SORE}
S_2 = aa? \text{ is NOT SORE}
```

Example 6.1.1 shows two regular expressions. The first one (S_1) is a SORE expression, but the second one (S_2) is not because there are two occurrences of a.

The iXSD algorithm supposes that the input set of XML documents is k-local and contains only content models expressible by single occurrence regular expressions.

6.1.1 Algorithm

The algorithm of iXSD consists of two steps — **iLocal** and **Reduce**. iLocal identifies all k-local content models and creates types of them. Reduce step merges similar-enough types.

For the needs of the algorithm we define several terms.

- Definition 6.1.3. We denote **paths(f)** for an XML fragment f to be a set of all labeled paths starting at root element in f.
- Definition 6.1.4. We denote **k-path** $p|_k$ of path p to be a path formed by the last k labels of path p. Two paths p and q are **k-equivalent** if $p|_k = q|_k$.

Example 6.1.2. XML fragment and paths

```
F :=
library>
<documents>
<book>
<title>Krakatit</title>
<author>Karel Čapek</author>
```

```
</book>
            <book>
                   <title>Big encyclopedia </title>
                   <author>Some author 1</author>
                   <author>Some author 2</author>
                   <summary>Some summary of the Big Encyclopedia</summary>
            </book>
            <article>
                   <title>Some technical article</title>
                   < author > Author </ author >
                   <summary>Summary of this technical article</summary>
            </article>
     </documents>
paths(F) = \{\lambda, \text{ library, library documents, library documents book, library documents book}\}
title, library documents book author, library documents book summary, library documents
article, library documents article title, library documents article author, library documents
article summary)
2-paths(F) = \{\lambda, \text{ library, library documents, documents book, book title, book author, book }\}
summary, documents article, article title, article author, article summary}
```

Example 6.1.2 shows a XML fragment and all paths and 2-paths.

Definition 6.1.5. We define **strings(f, p)**, where f is an XML fragment and p is a path, to be the a set of all names of element directly below an occurrence identified by the path p.

If the path p in the string(f, p) is a k-path we use the term **k-strings(f, p** $|_k$).

```
Example 6.1.3. K-string example
```

```
2-strings(F, documents book) = {title author, title author author summary} 
1-strings(F, author) = {\lambda, \lambda, \lambda, \lambda, \lambda}
```

Example 6.1.3 shows the usage of function string on the XML fragment from Example 6.1.2.

Now we have basic definitions and can proceed to the main algorithm.

```
Algorithm 6.5.3 iLocal
```

```
Types iLocal (int K, XMLFragments[] C) {
    var paths = paths(C);
```

```
var types = create type for each unique k-path from paths;
    foreach(type t in types) {
          //create single occurrence automata
          t.soa = iSOA(k-strings(C, t.kPath));
          //convert the automata to SORE
          t.regex = createSore(t.soa);
    Foreach(path (p,a) in paths) {//(p,a) consist of a path 'p' and a
label 'a'
           Type[p|_k].addTypeMapping(a, types[(p, a)|_k]);
    }
    return types;
}
Automata iSOA(string [][] labels) {
    var aut = create empty SOA;
    var uniqueNames = getUniqueNames(labels);
    aut.createVertices(uniqueNames);
    foreach (string[] labelSet in labels) {
          let labeSet have the form of (s<sub>1</sub>, s<sub>2</sub>, ..., s<sub>n</sub>)
          aut.connectVertices ((aut.start, s<sub>1</sub>), (s<sub>1</sub>, s<sub>2</sub>),...(s<sub>n</sub>, aut.out));
    return aut;
```

The iLocal - Algorithm 6.5.3 – creates types based on their K-path. Note that there will be more types than necessary. E.g. all empty elements with different k-paths will have different types, but they could easily have only a single type – empty. We will thus post-process the result of iLocal and merge the same types using the Minimalize algorithm.

```
Example 6.1.4. Ilocal results
```

Types generates by iLocal on F (Example 6.1.2) and k = 2:

 λ , library, library documents, documents book, document article, book title, book author, book summary, article name, article author, article summary

Example 6.1.4 shows the types that will be found on the XML fragment from Example 6.1.2. Note that e.g. types book title, book author, article name could be merged into the same type since they contain only text data.

```
Algorithm 6.5.4
                     Minimalize
```

```
Void minimalize(Types T, Type ignore, XMLFragments[] C) {
    while(exists Type t, s \in T, t \neq s \land t \neq ignore) {
          If (setsEqual(k-strings(C, t.kPath), k-string(C, s.kPath)) {
               foreach(Type k that contains mapping to t) {
                     k.changeMapping(a, s);
               T.removeType(t);
```

Example 6.1.5. Output of Minimalize

Minimalize on the result of Example 6.1.4 will return these types:

 λ , library, library documents, documents book, document article, book title

Example 6.1.5 shows the minimalization of equal types of iLocal algorithm from Example 6.1.4. Note that there is significantly less types now. All types with empty content were merged into a single type with kPath book title.

After running the iLocal and Reduce algorithms, we have set of types that are each unique. The next step - Reduce - will identify similar types and merge them. For that we will define the distance of types.

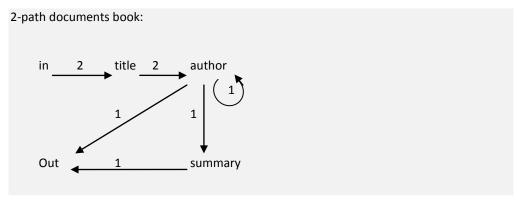
We have to modify the iSOA algorithm. Each edge will contain a number usage how many words from k-strings used this edge. Let as have a look on the adapted iSOA.

```
Algorithm 6.5.5
                  Adapted iSOA
   Automata iSOA(string [][] labels) {
```

```
var aut = create empty SOA;
var uniqueNames = getUniqueNames(labels);
aut.createVertices(uniqueNames);
foreach (string[] labelSet in labels) {
    let labeSet have the form of (s<sub>1</sub>, s<sub>2</sub>, ..., s<sub>n</sub>)
    foreach(edge e in {(aut.start, s<sub>1</sub>), (s<sub>1</sub>, s<sub>2</sub>),...(s<sub>n</sub>, aut.out)}) {
        if (aut.hasEdge(e)) {
            aut.edge[e].usage++;
        } else {
            add edge e to automata aut with usage 1.
        }
    }
}
return aut;
}
```

To determine the usage between two labels a and b of an Automaton A we use the function $supp_A(a,b)$.

Example 6.1.6. Example of adapted iSOA



Example 6.1.6 shows a SOA for content model of the type "documents book" with edges and their usages. The XML fragment is taken from Example 6.1.2. In that fragment there are two occurrences of the type "documents book", but only one contains summary and multiple authors.

Definition 6.1.6. Let A=(E,V) and B=(W,F) be two SOA. We define the normalized edit distance **dist** as follows:

$$dist(A,B) := \frac{\sum_{(a,b) \in E-F} supp_A(a,b)}{\sum_{(a,b) \in E} supp_A(a,b)} + \frac{\sum_{(a,b) \in F-E} supp_B(a,b)}{\sum_{(a,b) \in F} supp_B(a,b)}.$$

Definition 6.1.7. An XSD is a triple $D = (T, \rho, \tau)$ where T is a set of types, $\rho: T \longrightarrow Regex(X)$, where X is set of label names, and τ is mapping $(T \times X) \longrightarrow T$ that assign a type to a child element.

Definition 6.1.8. For an XSD $D = (T, \rho, \tau)$, let $elems_D(t)$ denote the set of all element names a for which $\tau(t, a)$ is defined. The set $reach_D(s, t)$ of pairs of types jointly reachable from (s, t) is the least set containing (s, t) such that $(x, y) \in reach_D(s, t)$ and $a \in elems_D(x) \cap elems_D(y)$ implies that $(\tau(x, a), \tau(y, a)) \in reach_D(s, t)$.

Intuitively, $reach_D(s,t)$ is the set of all pairs (x,y) for which there exists a path p such that $\tau(s,p) \to x$ and $\tau(t,p) \to y$.

In the next definitions we also use the function soa(t), that represents the result of adopted iSOA algorithm that we store for each type.

Definition 6.1.9. The edit distance $dist_D(s,t)$ between two inferred types is defined as

$$dist_D(s,t) \coloneqq max_{(x,y) \in reach_D(s,t)} dist(soa(x), soa(y)).$$

Now we have defined the edit distance of two types and can proceed to the algorithm Reduce that finds similar types and merges them.

Algorithm 6.5.6 Reduce

```
void Reduce(Types T, double E) {  var M = \{(s,t) \in T^2 | \ 0 < dist_D(s,t) < E\}  while (M is non-empty) {  foreach((s,t) in M) \{   foreach(x,y) in reach(s,t)) \{
```

```
 x.soa = x.soa \uplus y.soa; \\ y.soa = x.soa; \\ foreach(a in elems(y) - elems(x)) \{ \\ x.addTypeMapping(a, y.mapping[a]); \\ \} \\ foreach(a in elems(x) - elems(y)) \{ \\ y.addTypeMapping(a, x.mapping[a]); \\ \} \\ \} \\ recompute M = \{(s,t) \in T^2 | 0 < dist_D(s,t) < E\} \\ \} \\ \} \\ Foreach(type t in T) \{ \\ t.regex = createSore(t.soa); \\ \} \\ Minimalize(T); \\ \}
```

We demonstrate the work of the Reduce algorithm on an example.

Example 6.1.7. Reduce demonstration

```
Reduce on the result of Example 6.1.5 with E=0.5 will return these types: \lambda, library, library documents, documents book, book title. It merged types s = documents\ book \qquad \text{and} \qquad t = documents\ article since Dist(s,t) = \frac{1}{4}
```

6.1.2 Summary

The iXSD algorithm recognizes a single type grammar. It is able to identify types based on a definable context and not only on element names. The iXSD uses two parameters – k for the size of the context and E for the sensitivity for type merging.

7 Implemented solution

In previous chapters we analyzed and described a lot of algorithms. In this chapter we introduce our implementation for Schematron schema inferring.

Our goal is to infer a Schematron schema out of a set of XML documents. Our solution is divided into two parts – grammar inferring and Schematron schema generation. For the grammar inferring part we use the iXSD algorithm described in Chapter 6.1. For the Schematron schema generation part we use our three part algorithm from Chapter 5.

The reason for splitting our solution into two independent parts is because of the nature of Schematron. The inferred grammar can contain types that we are not interested in, or some types may not have been identified correctly. With our approach, the user can fix and simplify the inferred schema and thus gaining a better control of the output. Another advantage is that a user may choose a different inferring tool.

Our solution is written in C# over .NET Framework 3.5 as two separate command line applications. The usage is described in the appendix.

7.1 Data limitations

Since we use the iXSD algorithm, we expect that the data follow the two observations – locality and single occurrence. If the data will not support these two expectations, the result may be too general since the iXSD algorithm will always try to return SORE content models.

Our algorithm from Chapter 5 comes with two limitations on the input grammar. The first limitation – single type – is trivially fulfilled by the fact that the iXSD algorithm produces single type grammar. The second – determinism in derivation sequence – will be resolved by the k-local feature of the iXSD that will be used also in the context matching of our Schematron schema generation.

7.2 Usage of iXSD

In our solution we used the core of the iXSD algorithm as described in Chapter 6.1. The only difference from the intended usage of the iXSD is the form of the inferred grammar. We do not use XML Schema but a very simple form of grammar description. The Relax NG schema for inferred grammars can be found in the appendix.

7.2.1 Inferred grammar

The result of the step 1 of our solution is an XML document referenced as the inferred grammar. It contains two sets of definitions – types and elements.

The type definitions describe the whole inferred grammar. Each definition contains the description of its own content model, the names of child elements and their types. The section is similar to a Relax NG or XSD schema in the meaning that it defines all the hedges of the documents.

The other section - elements - contains constrains for content models of XML documents. Based on K ancestors it references a type that should be used to validate the content. This approach lets user to validate only a specific parts of XML documents and thus a more Schematron-like approach.

Relax NG schema for inferred grammar can be found on the CD and in the Appendix.

The second part of our solution – Schematron schema generation – uses constrains from elements.

7.3 Schematron schema generation

The Schematron schema generation consists of three parts: context matching, boundary rules and order check.

In this thesis we discussed several ways of context matching. Because of the locality observation of the iXSD algorithm, we choose the k-ancestor approach.

Although the inferred grammar of the iXSD algorithm should contain only SORE content models, our solution supports also simple multi-occurrence regular expressions. This support is limited as discussed in Chapter 5.

7.4 Experimental data sets

We used our solution on experimental data taken from real world. We present two data sets. Each set is presented in the same folder structure. It contains folder for grammars where all schemas and inferred grammars are stored and a folder for XML data.

The inferred schema (produced by step 1 of our solution) is named *InferredGrammar.xml*. The generated Schematron schema is named *schematronSchema.sch*. For all of our experimental data sets we use the default settings for grammar inferring (k=2, E=0.3).

Data set 1

This data set contains XML representation of a very common book – the Bible. We do not have any schema, just a single XML document. The XML document has a simple internal structure see Example 7.4.1. The full version of the XML document can be found on the CD.

Example 7.4.1. XML fragment of the Bible data set

Example 7.4.1 shows an XML fragment - the first verses of the first book of the Bible.

Example 7.4.2. Inferred grammar for Bible

```
<schema>
    <definitions>
           <definition name="chapter">
                 <oneOrMore>
                       <element name="verse" type="ValueOrEmpty" />
                 </oneOrMore>
           </definition>
           <definition name="ValueOrEmpty">
                 <empty />
           </definition>
           <definition name="book">
                 <oneOrMore>
                       <element name="chapter" type="chapter" />
                 </oneOrMore>
           </definition>
    </definitions>
    <elements>
           <element ofType="chapter">
                 <location>
                       <parent name="chapter">
                              <parent name="book" />
                       </parent>
                 </location>
           </element>
    </elements>
</schema>
```

In Example 7.4.2 we part of the inferred grammar for the first data set. The full version of the grammar can be found on the CD.

As we can see in Example 7.4.2, the inferred grammar for Bible is also simple. All content models are single occurrence and thus we should not have any difficulties in Schematron schema generation.

Example 7.4.3. Schematron schema for data set 1

```
<schema xmlns="http://purl.oclc.org/dsdl/schematron">
  <pattern>
```

```
<rule context="//book/chapter">
                   <assert test="count(verse) &gt;= 1">There must be at least 1 element(s)
"verse".</assert>
                   <assert test="(count(verse)) = count(child::*)">There are illegal
elements. Only elements "verse" are allowed</assert>
            </rule>
            <!--rules for checking regex regex "verse+"-->
            <rule context="//book/chapter/verse">
                   <assert test="following-sibling::*[1][self::verse] or not(following-</pre>
sibling::*)">Element "verse" can only be followed by "verse" or cannot be followed by any
other element</assert>
            </rule>
     </pattern>
     <pattern>
            <rule context="//chapter/verse">
                   <assert test="count(child::*) = 0">No children are allowed.</assert>
            </rule>
     </pattern>
</schema>
```

Example 7.4.3 shows part of the generated Schematron schema. The full version of the Schematron schema can be found on the CD.

The generated Schematron schema contains one pattern for each element definition in the inferred grammar. Each pattern consists of several rules constraining the corresponding grammar type.

Data set 2

In the second data set we initially had only XSD schema (*schema.xsd*) for NASC arrays. The XSD contains choices, sequences and types. There are more types than in the data set 1. Because the both the inferred grammar and the corresponding Schematron schema are too big we will show only small interesting XML fragments as examples. All the referenced files can be found on the CD.

Based on the XSD we generated two sample XML documents – the first with random choice and repetition and the second one without repetition.

The inferred grammar is bigger this time. It contains 23 types and about 130 element definitions. Schematron schema for this bigger grammar is also supplied

and it works. Note that there are some examples of multi occurrence content models. However for better performance the inferred grammar should be simplified.

Example 7.4.4. Complex definition from the inferred grammar for data set 2

```
<definition name="Source">
    <choice>
           <oneOrMore>
                 <element name="StockCode" type="ValueOrEmpty" />
           </oneOrMore>
           <group>
                 <element name="Individual" type="ValueOrEmpty" />
                 <choice>
                       <element name="Organism" type="ValueOrEmpty" />
                       <group>
                              <element name="IndivGeneChar" type="ValueOrEmpty" />
                              <optional>
                                    <element name="GeneticBackground"
type="ValueOrEmpty" />
                                                       </optional>
                       </group>
                 </choice>
           </group>
           <group>
                 <element name="invitroTreat" type="Other" />
                 <element name="CellLineSource" type="ValueOrEmpty" />
                 <optional>
                       <element name="Age" type="ValueOrEmpty" />
                 </optional>
           </group>
           <group>
                 <optional>
                       <element name="SeperationTechnique" type="Other" />
                 </optional>
                 <element name="CellLineSource" type="ValueOrEmpty" />
                 <optional>
                       <element name="Age" type="ValueOrEmpty" />
                 </optional>
           </group>
```

Example 7.4.4 is a typical example of a multi-occurrence content model. E.g. the type StockCode or IndivGeneChar is occurring more than once.

We can see some suspicious type definitions in the inferred grammar. We can also notice some multi-occurring content models. See Example 7.4.4. This is caused by a small set of input XML documents and their small variability and also by the complex type used to generate the data. Our implementation of the iXSD algorithm was not able to simplify enough the regex of this type. Thanks to this fact, we can demonstrate the ability of basic multi-occurrence support of our Schematron schema generation.

Example 7.4.5. Multi-occurrence support of Schematron schema generation

```
<!-- Symbol IndivGeneChar: -->

<!--Warning: support for multi-occurence symbols is not fully implemented-->

<rule context="//Extract/Source/IndivGeneChar[not(preceding-sibling::*)]">

<assert test="following-sibling::*[1][self::GeneticBackground] or not(following-sibling::*)">Element "IndivGeneChar" can only be followed by "GeneticBackground" or cannot be followed by any other element</assert>

</rule>

<rule context="//Extract/Source/IndivGeneChar[preceding-sibling::*[1][self::Individual]]">

<assert test="following-sibling::*[1][self::GeneticBackground] or not(following-sibling::*)">Element "IndivGeneChar" can only be followed by "GeneticBackground" or cannot be followed by any other element</assert>

</rule>
```

Shows part of the regex-checking rules for multi-occurring element IndivGeneChar.

Our algorithm detected two occurrences with different prefixes. However, notice

that the following asserts are identical and thus the generation process could be further improved.

In the *inferredGrammarSimplified.xml* we removed element definitions of type *ValueOrEmpty* and *Other*. Only this simple removal of the two most common (and trivial) element types reduced the number of element definitions to 26. Based on the user preferences the inferred grammar could be simplified further.

7.5 Conclusion

Our solution works on the most data from the real world – we use the iXSD algorithm. See Chapter 6.1 for more details about the properties of the real world data. However, we could see that both the inferred grammar and the generated Schematron schema are often bigger than necessary.

The most trivial comparison is by the file sized of the schemas of the second experimental data set: XSD Schema – 20kB, inferredGrammar - 23kB, inferredGrammarSimplified - 13kB, SchematronSchema – 71kb, SchematronSchemaSimplified - 51kB. We must note that the original XSD schema also contains comments and attributes definitions that are not contained in the inferredGrammar nor in the SchematronSchema.

Our implementation is a proof of concept that a Schematron schema can be generated for set of XML documents. For the real-world usage the generator should be optimized and the inferred grammar reduced.

We did not compare the effectiveness of the validation between Schematron and other languages, but based on the file sizes of the schemas we recommend that Schematron is used only for validation of some interesting parts of XML documents and not for the validation of the whole document.

There is another interesting feature of our implementation. We can see that the most rules come from the regex matching. If we could reduce their number the resulting Schematron schema would be greatly simplified. This could be done by two approaches – firstly we could use a different query language with a regex

support, secondly we could allow any-order groups in the regex definition and thus skipping the regex matching altogether.

8 Related work

There has been research already done on the field of XML schema inference. In this chapter we describe in short the most related work on this field. For a much bigger overview of XML inferring methods we recommend the [32].

8.1 Inferring xml schema definitions from xml data

Paper [30] analyses the properties of real world XML documents and defines two most common properties - locality and single occurrence. Based on those two properties it introduces the iXSD algorithm. Since we described this approach in Chapter 6.1, we will no redefine the whole algorithm again. We will only summarize the basic idea.

Locality property means that each content model depends only on the last K ancestors. Single occurrence states that content models consists only of single occurrence regular expressions (each terminal is present at most once). The iXSD algorithm identifies types based on the locality property and merges the similar types. The output is a single-type tree grammar in the form of an XSD.

8.2 Even an Ant Can Create an XSD

Paper [33] introduces the *Schema miner*. This approach generates an XSD. It is a heuristic approach and allows inferring elements with the same name but with a different structure. It is also able to infer unordered sequences in a content model.

This approach exploits the ACO (Ant Colony Optimization, [34], [35]), sk-string, (k,h)-context and MDL-principle. The ACO is a heuristics that is able to find a suboptimal solution. It uses "ants" that search the space S of possible solutions. Ants try to find an optimal solution; each found solution is evaluated by the MDL principle. Each ant does only predefined amount of steps before it dies. In each step an ant searches a subspace of S for a local suboptimum. Based on how good a found solution is, the ant gives a positive feedback – pheromones. The following iterations of other ant adjust their search based on the amount of pheromones.

SK-string method is used for finding and merging equivalent states. It is a more relaxed form of Nerode equivalence. The Nerode equivalence says that two states p

and q are equivalent if the sets of all paths leading to terminal states are equivalent. For the simplicity sk-string compares only s most probable k-strings. K-string returns only paths of the length K or shorter that lead to a terminal state.

Definition 8.1.1. A regular language L is k-contextual, if there exists a finite automaton A s.t. L = L(A) and for any two states p_k , q_k of A and all input symbols $a_1a_2...a_k$: if there are two states p_0 q_0 of A s. t. $\delta(p_0a_1a_2...a_k) = p_k$ and $\delta(q_0a_1a_2...a_k) = q_k$, then $p_k = q_k$.

Definition 8.1.2. A regular language L is k-contextual, if there exists a finite automaton A s.t. L = L(A) and for any two states p_k , q_k of A and all input symbols $a_1a_2...a_k$: if there are two states p_0 q_0 of A s. t. $\delta(p_0a_1) = p_1$, $\delta(p_1a_2) = p_2$, ..., $\delta(p_{k-1}a_k) = p_k$ and $\delta(q_0a_1) = q_1$, $\delta(q_1a_2) = q_2$, ..., $\delta(q_{k-1}a_k) = q_k$ then $p_i = q_i$ for every i s. t. $0 \le h \le i \le k$.

8.3 Automatic Construction of an XML Schema for a Given Set of XML Documents

Thesis [29] enhances the *Schema miner* from previous chapter and introduces the *Schema builder*. The aim of Schema builder is to allow user interaction and recognize inheritance between types. Another improvement is that Schema builder matches elements with different name but similar structure.

User can preview identified types and adjust their regular expressions. However, the main addition of the user interaction is the ability to define inheritance between types.

8.4 Optimization and Refinement of XML Schema Inference Approaches

Another work that builds upon paper [33] is [36]. The author focusses on the fact, that many XML documents have some schema, but that schema is outdated, invalid or not complete. He proposes a method of inferring an updated schema from the old one. The benefit of this approach is that the new schema is enforced not to deviate much from the old one.

Another goal of this work is to develop a finer MDL metric. The newly proposed MDL metric should prefer simpler schemas.

8.5 Efficient Detection of XML Integrity Constraints

It is common that XML data have some integrity constraints. Even if these constraints are known, there may be some XML documents that violate some of the constraints. The work [37] discusses the problem of correcting these violations with the least modification as possible to the input documents.

The author introduces repair groups for different types of violations. Each repair action from a repair group is weighted and the least invasive is chosen. Another aspect of the this work is that the algorithm allows user input.

9 Conclusion

This thesis has brought a way to infer a Schematron schema for a set of XML documents. We have introduced Schematron in deeper, because it uses a different way of XML validation – it uses rules instead of grammar validation. Schematron supports more query languages, we chose XPath 1.0, since the support from third parties implementations of Schematron validators is the most common for XPath 1.0.

To our best knowledge, there has not been much work on automatic Schematron schema generation. Because of this fact we focused on analyzing and describing different ways of transforming a single type grammar to Schematron rules. This is the main part of this thesis and more future work can be based on it.

Since there have been works on automatic XML schema inferring (e.g. [28] or [29]), we reduced the analysis of existing inferring methods to a single representative – the iXSD algorithm. We used the iXSD algorithm later in our implementation.

Our implementation consists of grammar inferring part and of a Schematron schema generation part. User interaction is supported, since the user can modify the inferred simple grammar description or even write its own.

At the end we show some experimental results.

9.1 Future work

In this thesis there are some areas that we did not discuss at all or only a little. Some new areas came up as we proceeded with our analysis. These areas can bring new results and improve the current results. We will try to describe them in short in the following paragraphs.

One of the main areas that have not been touch is negative examples handling. Schematron (in contrast to other major validation languages) is able to express and check negative constraints. Current inferring methods use only positive examples. It would be interesting to be able to define negative constraints.

Schematron supports more query languages. We used XPath 1.0 since it is widely supported. We were limited by the use of XPath 1.0 in algorithms mainly because of the lack of regex support. However, other query languages can work better – like XPath 2.0. They bring new possibilities to match elements and thus they could greatly improve and simplify our algorithms.

There is another a way to reduce the number of generated rules and simplify the Schematron schema - by introducing any-order alternative for a group (like XS:any in XML Schema). In current implementation the majority of generated rules are for regex checking and thus, for unordered content models, these rules could be left out.

Our algorithm suggests a way to handle multi-occurrence content models with the help of prefix automata. However, this method is not fully completed since it does not handle all cases – mainly the length of repeated loops. Also there is some place to improve the generated queries and simplify them.

Lastly, the whole Schematron schema is not optimized. It can query multiple times the same elements or on the other hand uses too much variables. We think that this could be improved. Also the generated schema is too big and not all elements must be checked. The inferred grammar could be automatically optimized.

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11 Appendix - Content of the CD

The CD is part of this thesis. It contains this text, implementation, data sets and Relax NG schema for inferred grammar. Implementation is divided into two projects of Visual Studio 2010 – iXSD implementation and Schematron schema generator. Experimental data set contains data sets and also an Ant build file for running Schematron schemas on the input XML documents.

- content.txt text of this chapter
- text A directory with the pdf file with the text of this thesis
- src A directory with sources for our implementation and Relax NG schema for the inferred grammars.
- bin A directory with binaries of our implementation
- experimental data A directory for experimental data sets

12 Appendix Program usage

In this chapter we describe the usage of our implemented solution. The solution is divided into two parts iXSD.exe and SchemaGenerator.exe.

For help, run any program with the "-h" parameter.

Both binaries require RegularExpression.dll to be present in the run content and support for .NET framework 3.5.

12.1 iXSD

The iXSD.exe infers the grammar out of the input set of XML documents and generates the inferred grammar. The recognized parameters are:

```
Usage: [-h] [-k INTEGER] [-e DOUBLE] [-o OutputFile] (inputFile)*
Where:
```

- -h prints help and terminates
- -k is the number of ancestors to identify a type.
- -e is the number (0-1.0) for merging similar types (see Chapter 6.1).
- -o is the name of created output file. If not provided, standard output will be used
- Any following parameters are considered to be names of input XML documents

There must be provided at least one filename. All other parameters are optional.

12.2 Schematron Generator

The binary takes the inferred grammar (most likely from the iXSD part) and generates Schematron schema out of it. The recognized parameters are:

```
Usage: [-h] [-i inputFile] [-o OutputFile]
```

Where:

- -h prints help and terminates
- -i specifies the location of inferred grammar. If not provided standard input is used.

• -o specifies the location for the generated Schematron schema. If not provided, schema is printed to standard output.

All parameters are optional.

13 Appendix - attachments

Example 12.1.1. Relax NG schema for inferred grammar

```
<?xml version="1.0" encoding="utf-8"?>
<grammar
    datatypeLibrary="http://www.w3.org/2001/XMLSchema-datatypes"
    xmlns="http://relaxng.org/ns/structure/1.0"
    xmlns:a="http://relaxng.org/ns/compatibility/annotations/1.0">
    <start>
           <element name="schema">
                 <group>
                       <element name="definitions">
                              <zeroOrMore>
                                    <element name="definition">
                                          <ref name="definition"/>
                                    </element>
                              </zeroOrMore>
                       </element>
                       <element name="elements">
                              <zeroOrMore>
                                    <element name="element">
                                          <ref name="element"/>
                                    </element>
                              </zeroOrMore>
                       </element>
                 </group>
           </element>
    </start>
    <define name="definition">
           <attribute name="name">
                 <text/>
           </attribute>
           <ref name="regex"/>
    </define>
    <define name="regex">
           <choice>
                 <element name="empty">
                       <empty/>
```

```
</element>
            <element name="element">
                  <attribute name="name">
                         <text/>
                  </attribute>
                  <optional>
                         <attribute name="type">
                               <text/>
                         </attribute>
                  </optional>
            </element>
            <element name="optional">
                  <ref name="regex"/>
            </element>
            <element name="zeroOrMore">
                  <ref name="regex"/>
            </element>
            <element name="oneOrMore">
                  <ref name="regex"/>
            </element>
            <element name="choice">
                  <group>
                         <ref name="regex"/>
                         <oneOrMore>
                               <ref name="regex"/>
                         </oneOrMore>
                  </group>
            </element>
            <element name="group">
                  <group>
                         <ref name="regex"/>
                         <oneOrMore>
                               <ref name="regex"/>
                         </oneOrMore>
                  </group>
            </element>
      </choice>
</define>
```

```
<define name="element">
           <attribute name="ofType">
                  <text/>
           </attribute>
           <element name="location">
                  <ref name="location"/>
           </element>
    </define>
    <!-- Location serves to locate elements in XML document and to identify their type
without the need to define grammar for the whole XML-->
    <define name="location">
           <element name="parent">
                  <choice>
                        <group>
                               <attribute name="name">
                                     <text/>
                               </attribute>
                               <optional>
                                     <ref name="location"/>
                               </optional>
                        </group>
                        <element name="none">
                               <empty/>
                        </element>
                  </choice>
           </element>
    </define>
</grammar>
```

Relax NG schema for our inferred grammar.