3 XML Data Management and Bioinformatics applications

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using material from
- Alan Robinson, (recommended ! http://industry.ebi.ac.uk/~alan/XMLWorkshop/)
- Silverschatz and M. Sapossnek .

3.1 Introduction

- Formats: trivial but very important problem
  Example: sequence formats .
  Details: .... .
- Infinitely many ways to structure data
  ⇨ Basic issue: processing data
  not a real issue: human readibility
- Needed: standardized way of representation
- Retrieving data from MB databases: yet another example

http://www.ebi.ac.uk/cgi-bin/dbfetch r1 r2 r3

What is XML?

- Acronym for eXtensible Markup Language
- Syntax for structuring data and documents in human-readable form
- THE "Syntax of the WEB"
- Meta language for defining data description languages called applications, e.g. GAME, BSML, ...
- Basis for many extensions
  - Namespaces
  - Stylesheets
  - Hyperlinks
  - Schemata
- Standardized by W3C
  http://www.w3.org/TR/REC-xml

What XML is NOT..

- No protocol
  - Language for describing data
  - Used as data format in protocols
  - Protocols may be syntactically defined by XML
- No programming language

but
  - XML documents may contain code fragments
  - New languages allow for XML – code as part of the language (Xen, a MS extension of C#)
  - Some XML extensions with superimposed PL semantics, rule semantics in XSLT
- No magic semantics
  - Interpretation by humans, applications, standards derived from XML

Why XML?

- … not a question any more, since widely adopted
- Simple
- Extensible
- Easy to process
- Easy to generate
- Data interchange critical for networked applications

"XML will be the ASCII of the Web:
basic, essential, unexciting"

Tim Bray

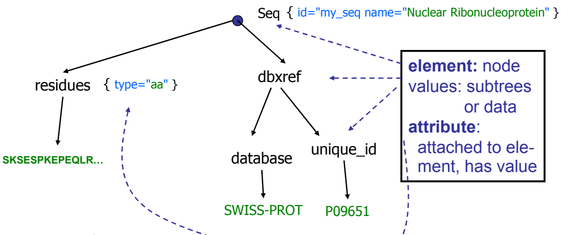
... it is already

XML markup: example

```
<?xml version="1.0"?>
<seq id="my_seq" name="NUCLEAR RIBONUCLEOPROTEIN">
  <dbxref>
    <database>SWISS-PROT</database>
    <unique_id>P09651</unique_id>
  </dbxref>
  <residues type="aa">
SKSESPKEPEQLRKLFIGGLSFETTDESLRSHFEQWGTLTDCVVMRDPNTKRS
RGFGFVTYATVEEVDAAMNARPHKVDGRVVEPKRAVSREDSQRPGAHLTVKKI
FVGGIKEDTEEHHLRDYFEQYGKIEVIEIMTDRGSGKKRGFAFVTFDDHDSVD
KIVIQKYHTVNGHNCEVRKALSKQEMASASSSQRGRSGSGNFGGGRGGGFGGN
DNFGRGGNFSGRGGFGGSRGGGGYGGSGDGYNGFGNDGGYGGGGPGYSGGSRG
YGSGGQGYGNQGSGYGGSGSYDSYNNGGGRGFGGGSGSNFGGGGSYNDFGNYN
NQSSNFGPMKGGNFGGRSSGPYGGGGQYFAKPRNQGGYGGSSSSSSYGSGRRF
  </residues>
</seq>
```

XML example

- Graphical representation



element: node
values: subtrees or data
attribute: attached to element, has value

XML documents
- tree structured
- Data and metadata in the same document

(as opposed to RDBS / ODBS / ..)

Another Example

- Semantics??

```
<?xml version="1.0"?>
<pd>
  <b>
    <d>22</d>
    <m>5</m>
    <y>70</y>
  </b>
  <ec>green</ec>
  <pc>CB2 2EZ</pc>
</pd>
```

```
<?xml version="1.0"?>
<pd>
  <b>
    <d>22</d>
    <m>5</m>
    <y>70</y>
  </b>
  <ec>green</ec>
  <pc>CB2 2EZ</pc>
</pd>
```

c.f Alan Robinson

Third example

```
<Orders>
   <SalesOrder SONumber="12345">
        <Customer CustNumber="543">
           <CustName> ABC Industries</CustName>
           <Street> 123 Main St.</Street>
           <City>Chicago</City>
            ....
        </Customer>
       <Line LineNumber="1">
           <Part PartNumber="123">
              <Description>
                 <p><b> Turkey wrench:</b><br />
                 Stainless steel, one-piece construction,
                 lifetime guarantee.</p>
              </Description>
              <Price>9.95</Price>
           </Part>
           <Quantity>10</Quantity>
        </Line>
        .......
    </SalesOrder>
 </Orders>
```

relational schema?

XML Usage

- Basic types of XML usage

  Document centric (document oriented)
  - structuring a digital document, including logical layout
  - primary focus of SGML - predecessor of XML
- Data centric
  - Description of data in a self describing form for later processing
- Distinction ?
  - not always clear
  - data centric: database / query oriented
  - document: layout ... but on a logical level

Document centric XML documents: example

```
<Product>
  <Name>Variabler Maulschlüssel</Name>
   <Developer> Full Fabrication Labs, Inc. </Developer>
   <Summary> Großer, verstellbarer Schraubenschlüssel</Summary>
   <Description>
    <Para>Der Engländer besteht aus erstklassigem Stahl und
    besitzt einen gummierten Handgriff. Die Maulgröße liegt
    zwischen 0 und 32 mm.   </Para>
    <Para>Sie können.....   </Para>

   <List>
    <Item> <Link URL="Order.html"> Bestellen </Link></Item>
    <Item> <Link URL="Wrenches.htm"> Andere Werkzeuge ansehen
           </Link> </Item>
    <Item> <Link URL="catalog.zip"> Den Katalog herunterladen
    </Link> </Item>
   </List>
   <Para> Der Schraubenschlüssel kostet 15.33 Euro inkl. MWSt. Wenn
          Sie jetzt bestellen, erhalten Sie zusätzlich unsere
          wertlose Hobbybastler-Fibel.</Para>
   </Description>
</Product>
```

Typical:Long text elements

Note: Layout of logical elements can be defined independently!

Document or data centric?

Insulin receptor sequence

3.2 XML Syntax

- One, and only one, root element
- Sub-elements must be balanced and properly nested

  <TAG> <TAG2> ... </TAG2> </TAG>
- Attributes are optional
- Attribute values must quoted <TAG a1="val">...
  - No other data type than 'String'
- Empty tag: <Leer/>, comment <!-- ..... -->
- XML is case-sensitive
  - `<tag>` and `<TAG>` are not the same type of element
- Special characters for <,>,...." ⇨ &lt; &gt; ...., &quot
- Document always begins with XML version:

  <?xml version="1.0"?>

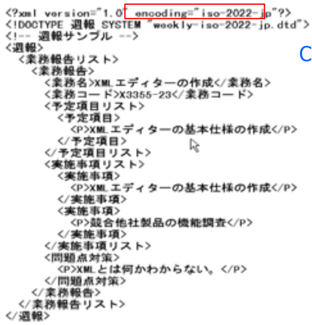
XML Attributes vs Elements

- Distinction between subelement and attribute
  - In the context of documents:
    - attributes are part of markup
    - subelement contents part of the basic document content
  - In the context of data representation:
    difference not clear, but confusing
    - Same information can be represented in two ways

```
<seq id="my_seq" name="NUCLEAR RIBONUCLEOPROTEIN">
    ....
</seq>          or...
<seq>
      <id>  my_seq       </id>
     <name> NUCLEAR RIBONUCLEOPROTEIN </name>
  ...
</seq>
```

Suggestion: use attributes for identifiers of elements
use subelements for contents

Correctness?



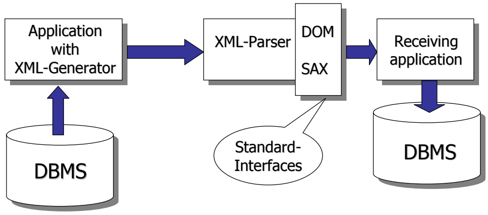
```
<?xml version="1.0" encoding="iso-2022-jp"?>
<!DOCTYPE 週報 SYSTEM "weekly-iso-2022-jp.dtd">
<!-- 週報サンプル -->
<週報>
  <業務報告リスト>
    <業務報告>
      <業務名>XMLエディターの作成</業務名>
      <業務コード>X3355-23</業務コード>
      <予定項目リスト>
        <予定項目>
          <P>XMLエディターの基本仕様の作成</P>
        </予定項目>
      </予定項目リスト>
      <実施事項リスト>
        <実施事項>
          <P>XMLエディターの基本仕様の作成</P>
        </実施事項>
        <実施事項>
          <P>競合他社製品の機能調査</P>
        </実施事項>
      </実施事項リスト>
      <問題点対策>
        <P>XMLとは何かわからない。</P>
      </問題点対策>
    </業務報告>
  </業務報告リスト>
</週報>
```

Correct or not correct ?

- Different encodings
- specified by encoding attribute

How to use XML data?

- Basic Idea



How does application know about
- syntactical correctness
- data semantics ?

DTD and XML schema

- Two ways to define the "schema" of an XML doc
  - Document Type Definition
  - XML Schema
- Document Type Definition (DTD)
  - Defines syntactic structure of a class of XML docs
  - Syntax
    - which elements? Attributes?

    <!ELEMENT elem (subelement-spec)>

    <!ATTLIST elem (attribute-specs) >
    - Nesting ⇨ tree structure
    - optional / mandatory elements

Correctness of XML documents

- Syntactic correctness
  - Conformance to XML syntax
  - Document structured according to XML syntax is well-formed Compare Syntax checker for program
- Semantic correctness
  - Given Meta level description of XML documents: Document Type Definition (DTD) or XML Schema
  - Document is valid with respect to DTD (Schema) if all definitions and restrictions have been fulfilled
  - No DTD ⇨ applications must know, what is meant

But: what is THE semantics of an XML doc?

Example DTD

```
<?xml version="1.0" encoding="US-ASCII"?>
<!DOCTYPE seq [
 <!ENTITY % shape "(rect|circle|poly|default)">
 <!ELEMENT seq (dbxref*, residues?) >
  <!ATTLIST seq     id     ID     #REQUIRED
                    name   CDATA  #IMPLIED
                    length CDATA  #IMPLIED >
 <!ELEMENT residues (#PCDATA)>
  <!ATTLIST residues  type  (dna | rna | aa)
#REQUIRED>...
]>
```

Entity:
simplest form abbreviation, here: enumeration

Nesting of elements:
“|” : alternatives
“+” : 1 or more occurrences
“*” : 0 or more occurrences
"?" 0 or one

Attribute spec:
#REQUIRED, default val, #IMPLIED (= optional)
enumeration type

CDATA: not parsed, #PCDATA : parsed char data

DTD attribute ID

- At most one attribute of type ID per element
- ID attribute value of each element in an XML document must be distinct
  - ID attribute value is object identifier
- attribute of type IDREF must contain the ID value of an element in the same document
- attribute of type IDREFS contains a set of (0 or more) ID values. ID value must contain the ID value of an element in the same document
- ID, IDREF, IDREFS do not designate a particular domain (no type!)

DTD declaration

External DTD-declaration

<?xml version="1.0">
<!DOCTYPE BSML PUBLIC
"HTTP://LABBOOK.COM/DTD/BSML3_1.DTD">
<Sequence ...> ... </Sequence>

Bioinformatic Sequence Markup Language

Internal DTD-declaration

<!DOCTYPE custDesc [<!ELEMENT custDesc (#PCDATA)>]>
<custDesc> consumer rights protagonist </custDesc>

Mixed usage

<!DOCTYPE bank SYSTEM "http://www.x-ag.de/banks.dtd" [
<!ATTLIST bank _Descr CDATA #REQUIRED>
]>
<bank _Descr=" mostly private customers and ATM"> ... </bank>

XLink / XPointer

- Link to external resources (documents, images...)
- XML link
  - URL ⇒ a resource
  - URL + XPointer ⇒ sub-resource of URL
  - XPointer ⇒ sub-resource of current URL

Example:

```
<mylink xmlns:xlink="http://www.w3.org/1999/xlink" xlink:type="extended">
 <myresource xlink:type="locator"
   xlink:href="students.xml#Fred" xlink:label="student"/>
 <myresource xlink:type="locator"
      xlink:href="teachers.xml#Joe" xlink:label="teacher"/>
 <myarc xlink:type="arc" xlink:from="student" xlink:to="teacher"/>
</mylink>
```

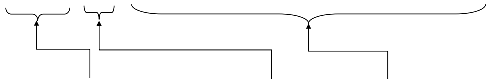
??

cf the tutorial on XLink / XPointer http://www.brics.dk/~amoeller/XML/linking/

XML Namespaces

- Part of XML’s extensibility
- Allow autonomous users to differentiate between tags with the same name (using a prefix)
  - Resolves naming conflicts
  - Allows multiple XML documents from multiple authors to be merged

```
xmlns:bk = “http://www.example.com/bookinfo/”
```



Namespace declaration

Prefix

URI (URL)

Namespace

- Examples

```
<BOOK xmlns:bk=“http://www.bookstuff.org/bookinfo”>
   <bk:TITLE>All About XML</bk:TITLE>
   <bk:AUTHOR>Joe Developer</bk:AUTHOR>
   <bk:PRICE currency=‘US Dollar’>19.99</bk:PRICE>
```

- No prefix: all elements belong to same namespace

```
<BOOK xmlns=“http://www.bookstuff.org/bookinfo”>
   <TITLE>All About XML</TITLE>
   <AUTHOR>Joe Developer</AUTHOR>
```

XML Schema

- XML Schema (XSD): much more expressible Schema language compared to DTD schemas
  - Typing of values
    - E.g. integer, string, etc
    - constraints on min/max values
  - User defined types
  - specified in XML syntax, unlike DTDs
    - More standard representation, but verbose
  - namespace support
  - Many more features
    - List types, uniqueness and foreign key constraints, inheritance
      Ability to map to RDB,…
- Significantly more complicated than DTD syntax
- Use of XSD recommended

XSD example

(from Silverschatz)

```
<xsd:schema xmlns:xsd="http://www.w3.org/2001/XMLSchema">
<xsd:element name=“bank” type=“BankType”/>
<xsd:element name=“account”>
   <xsd:complexType>
       <xsd:sequence>
           <xsd:element name=“account-number” type=“xsd:string”/>
           <xsd:element name=“branch-name”      type=“xsd:string”/>
           <xsd:element name=“balance”
   type=“xsd:decimal”/>
       </xsd:sequence>
   </xsd:complexType>
</xsd:element>
<!-- definitions of customer and depositor  should go in here-->
<xsd:complexType name=“BankType”>
   <xsd:sequence>
    <xsd:element ref=“account”   minOccurs=“0”
   maxOccurs=“unbounded”/>
    <xsd:element ref=“customer” minOccurs=“0”
   maxOccurs=“unbounded” />
     <xsd:element ref=“depositor” minOccurs=“0”
   maxOccurs=“unbounded”/>
    </xsd:sequence>
</xsd:complexType>
</xsd:schema>
```

XML Schema

EML XML – Schema for sequences

```
<?xml version="1.0" encoding="UTF-8"?>
<!--
*****************************************************************************
XML Schema for the components of an EMBL sequence record
Version 1.0, 15 March 2005
 by Vincent Lombard
*****************************************************************************
The EMBL Nucleotide Sequence Database (also known
as EMBL-Bank) constitutes Europe's primary nucleotide
sequence resource.
This XML Schema describes the structure of entries in the EMBL database.
These entries incorporate DNA or RNA sequences.......
-->
<xs:schema xmlns:ebi="http://www.ebi.ac.uk/xml" xmlns:xs="http://www.w3.org
          <xs:complexType name="entryType">
                 <xs:sequence> ..........
        </xs:complexType name="entryType">
```

XSD, not MB sequence!

XML Schema

- Based on an extensible type concept
- built-in types: `double, float...` (primitive), `integer -> nonPositiveInteger,`
  `-> nonNegativeInteger ..`
  `-> long, ...`
- simple types: defined by value type, representation and restrictions,
  do not have attributes or child elements

```
<xs:simpleType name = seqType>
     <xs:restriction base="xs:NMTOKEN">
          <xs:enumeration value="single"/>
          <xs:enumeration value="join"/>
          <xs:enumeration value="order"/>
     </xs:restriction>
</xs:simpleType>
```

- Complex types:
  - used to define substructures

    compare element structuring in DTD

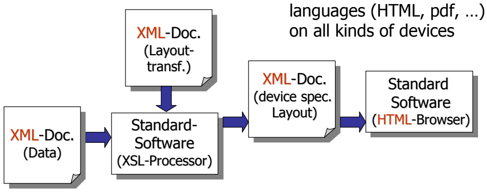
```
<xs:complexType name="locationtype">
  <xs:annotation>
   <xs:documentation>Type can be either a single a join or an order
   </xs:documentation>
  </xs:annotation>
  <xs:sequence>
          <xs:element name="locationElement"
               type="locationElementType" maxOccurs="unbounded"/>
  </xs:sequence>
  <xs:attribute name="type" use="required">
          <xs:simpleType>
                    <xs:restriction base="xs:NMTOKEN">
                              <xs:enumeration value="single"/>
                              <xs:enumeration value="join"/>
                              <xs:enumeration value="order"/>
                    </xs:restriction>
          </xs:simpleType>
  </xs:attribute>
  <xs:attribute name="complement" type="xs:boolean" use="required"/>
</xs:complexType>
```

3.5 Using XML

- Data exchange ☑
- Data management:
  - Store, retrieve, query large document sets efficiently
    - Today's solutions:
      - Mapping to RDB / ORDB / OODB
      - "Native" XML data management (not necessarily very different from storing in conventional DB)
- Standardized data description: different extensions and applications
  - Bioinformatic Sequence Markup Language (BSML)
  - MathML, Scalable Vector Graphics (SVG)
    .. and many, many more
  - Ressource Description in the web (RDF)
    Semantic Web (whatever that means..)
- Logical / Physical layout

Using XML: Logical – Physical Layout

- Layout of documents?
  - XML documents specify logical structure
  - Layout structure needed for output
    - Use transformation language to describe device specific transformations


XML-Doc. (Layout-transf.)
XML-Doc. (Data)
Standard-Software (XSL-Processor)
XML-Doc. (device spec. Layout)
Standard Software (HTML-Browser)

Transformation into all kinds of languages (HTML, pdf, ...) on all kinds of devices

XML transformation

- XSLT: The language used for converting XML documents into other forms
- Describes how the document is transformed
- Expressed as an XML document (.xsl)
- Template rules
  - Patterns match nodes in source document
  - Templates instantiated to form part of result document
- XPath for querying, sorting, etc.
- XSL-FO language for describing layout

XSL = XSLT + XPATH + XSL-FO

XML transformation: example (1)

- Document

```
<sales>
  <summary>
    <heading>Scootney Publishing</heading>
    <subhead>Regional Sales Report</subhead>
    <description>Sales Report</description>
  </summary>
  <data>
    <region>
      <name>West Coast</name>
      <quarter number="1" books_sold="24000" />
      <quarter number="2" books_sold="38600" />
      <quarter number="3" books_sold="44030" />
      <quarter number="4" books_sold="21000" />
    </region>
    ...
  </data>
</sales>
```

XML transformation: example (2)

- XSL style sheet - mapping to HTML

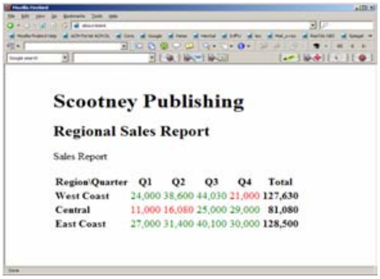
```
<xsl:param name="low_sales" select="21000"/>
<BODY>
 <h1><xsl:value-of select="//summary/heading"/> </h1>
 ...
 <table><tr><th>Region\Quarter</th>
   <xsl:for-each select="//data/region[1]/quarter">
     <th>Q<xsl:value-of select="@number"/></th>
   </xsl:for-each>
   ...
   <xsl:for-each select="//data/region">
   <tr><xsl:value-of select="name"/></th>
    <xsl:for-each select="quarter">
     <td><xsl:choose>
       <xsl:when test="number(@books_sold &lt;= $low_sales)">
         color:red;</xsl:when>
       <xsl:otherwise>color:green;</xsl:otherwise></xsl:choose>
     <xsl:value-of select="format-number (@books_sold,'###,###')"
       /> </td>
   ...
   <td><xsl:value-of
          select="format-number(sum(quarter/@books_sold),
                  '###,###')"/>
```

XPath expression

XPath: query language on doc trees

XML transformation: example (2)

- The result



Scootney Publishing

Regional Sales Report

Sales Report

Region\Quarter	Q1	Q2	Q3	Q4	Total
West Coast	24,000	38,600	44,030	21,000	127,630
Central	11,000	16,080	25,000	29,000	81,080
East Coast	27,000	31,400	40,100	30,000	128,500

Still to come....

- XML in bioinformatics (overview of activities)

- XPath, XQuery
- XML data management :

  Next generation data management system for molecular biology?

- (Similarity search in XML-DBS)