StatDataML—An XML Format for Statistical Data

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Abstract

In order to circumvent common difficulties in exchanging statistical data between heterogeneous applications (format incompatibilities, technocentric data representation), we introduce an XML-based markup language for statistical data, called StatDataML. After comparing StatDataML to other data concepts, we detail the design which borrows from the language S, such that data objects are basically organized as recursive and non-recursive structures, and may also be supplemented with meta-information.

1 Introduction

Data exchange between different tools for data analysis and data manipulation is a common problem: different applications use different and often proprietary and undocumented formats for data storage. Import/export filters are often missing or insufficient, and if ever, focus on technical aspects (like storage modes and floating point specifications) in spite of supporting conceptional representation issues (like scales or representation of categorical data). The currently high costs for data exchange hence could be significantly reduced by the use of a well-defined common data exchange standard, if only because software packages would just need to provide one single mechanism.

The aim of this paper is to introduce such a data exchange standard for statistical data: the XML-based markup language StatDataML. The design borrows from the language S (see e.g., Chambers, 1998), such that data objects are basically organized as recursive structures (lists) and non-recursive structures (arrays), respectively. Additionally, each object can have an attached list of properties (corresponding to S attributes), providing storage of meta-information.

2 Requirements on Statistical Data

Statisticians need a data format which is both flexible enough to handle all different kinds of statistical data (from time series to decision trees), and specialized enough to incorporate statistical notions like scales and factors. Such a data format should feature:

- special symbols for infinities and undefined values
- special symbols for missingness (“not available”)
- logical data
- categorical data (unordered, ordered or cyclic)
- numeric data (in the storage modes integer, real and complex)
- character data (strings)
- date/time information
- vectors (objects with elements of the same type)
- lists (objects with—possibly different—elements of any type)

Vectors should be indexable arbitrarily—in order to build matrices or multidimensional arrays. Lists allow for complex and even recursive structures (for they can contain lists again).

Table 1 compares some software products regarding these criteria: two families of mathematical programming languages (Splus/R and Matlab/Octave), statistical software (SPSS, SAS, Minitab) and spreadsheets (Excel, StarCalc, Gnumeric). In spreadsheets and Matlab/Octave, nominal data can only be represented by strings. Arrays of arbitrary dimension are supported by Splus/R and Matlab only. Complex numbers are only supported by Splus/R and Matlab/Octave. The latter cannot handle missingness. IEEE special values are not supported by Excel, StarCalc, SPSS, SAS and Minitab.

---

1 See Temple Lang & Gentleman (2001) for a more specific approach representing S objects in XML.
2 like days of a week
3 For Splus see: www.insightful.com
4 For R see: Ihaka & Gentleman (1996) and www.R-project.org
5 For Matlab see: www.mathworks.com
6 For Octave see: www.octave.org
7 For SPSS see: www.spss.com
8 For SAS see: www.sas.com
9 For Minitab see: www.minitab.com
10 For Excel see: www.microsoft.com
11 For StarCalc see: www.staroffice.com and www.openoffice.com
12 For Gnumeric see: www.gnumeric.org
Table 1: Data representation capabilities of different software packages

<table>
<thead>
<tr>
<th></th>
<th>R/Splus</th>
<th>Matlab</th>
<th>Octave</th>
<th>Excel/StarCalc</th>
<th>Gnumeric</th>
<th>SPSS</th>
<th>SAS</th>
<th>Minitab</th>
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<td>yes</td>
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<td>no</td>
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<td>no</td>
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<td>yes</td>
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</tr>
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</tr>
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<td>no</td>
<td>no</td>
<td>no</td>
</tr>
</tbody>
</table>

3 StatDataML

3.1 StatDataML is XML

For “statistical data” one would usually think of such things as tabular data, time series objects, responses and regressors or contingency tables. Programs that produce such data store it on disk, using either a binary format or a text format. StatDataML files are XML files, thus ordinary text files, with extension .sdml, containing several XML elements (so called tags), which can be formally described with a special data definition language (DTD)—see the World Wide Web Consortium (2000) recommendation. In the following, we will go through the rules in the StatDataML.dtd file.

3.2 The File Header

```xml
<!ELEMENT StatDataML (description?, dataset?)>
```

The top level StatDataML element contains one description and one dataset element, each optional. It should contain the StatDataML namespace:

```xml
<StatDataML xmlns="http://www.ci.tuwien.ac.at/StatDataML">
...
</StatDataML>
```

3.3 The description element

```xml
<!ELEMENT description (title?, source?, date?, version?,
comment?, creator?, class?, properties?)>
```

```xml
<!ELEMENT title (#PCDATA)>
<!ELEMENT source (#PCDATA)>
<!ELEMENT date (#PCDATA)>
<!ELEMENT version (#PCDATA)>
<!ELEMENT comment (#PCDATA)>
<!ELEMENT creator (#PCDATA)>
<!ELEMENT class (#PCDATA)>
```
The description element is used to provide meta-information about a dataset that is typically not needed for computations on the data itself. It consists of eight elements: title, source, date, comment, version, creator and class are simple strings (PCDATA), whereas properties is a list element (see next section). date should follow the ISO 8601 format (see below). The creator element should contain knowledge about the creating application and the StatDataML implementation. properties offers a well-defined structure to save application-based meta-information, and, finally, the class element will contain the class name, if any. There are some discussions about meta data in statistics\textsuperscript{13}: one could think of extending the description element in such that extended information with logical markup can be stored.

3.4 The dataset element

We define a dataset element either as an array or as a list. We use arrays and lists as basic “data types” in StatDataML because every data object in statistics can be decomposed into a set of arrays and lists (as in Splus/R, or like the corresponding arrays and cell-arrays in Matlab). The basic property of a list is its recursive structure, in contrast to arrays which are always non-recursive. If one thinks about data as a tree, lists would be the branches and arrays the leaves.

3.4.1 Lists

A list contains three elements: dimension, properties and listdata:

```xml
<!ELEMENT list (dimension, properties?, listdata)>
<!ELEMENT listdata (list | array)*)
<!ELEMENT dimension (dimm*)>
<!ELEMENT dim (e*)>
<!ATTLIST dim size CDATA #REQUIRED>
```

The dimension element contains one or more dim tags, depending on the number of dimensions. Each of them has size as a required attribute, and may optionally contain up to size names, specified with <e>...</e> tags. Note that arrays, like the whole dataset, can also have additional properties attached, corresponding, e.g., to attributes in S. In fact, the name “properties” was chosen because the name “attribute” is already used in XML itself. The listdata element may either contain arrays (with the actual data), or again lists, which allows for complex and even recursive structures.

3.4.2 Arrays

```xml
<!ELEMENT array (dimension, properties?, (data | textdata))>
```

Arrays are blocks of data objects of the same elementary type with dimension information used for memory allocation and data access (indexing). The first two elements, dimension and properties, are identical to lists, only the listdata block is replaced by the data (or textdata) element which contains the data itself.

The data tag

```xml
<!ELEMENT data (e|ce|na)*)
<!ATTLIST data
  true CDATA "1"
  false CDATA "0"
  type (logical|nominal|numeric|character|datetime) "character"
  mode (unordered|ordered|cyclic|integer|real|complex) #IMPLIED>
```

\textsuperscript{13}e.g., \url{http://www.gla.ac.uk/External/RSS/RSScomp/metamtg.html}
If data is used (especially recommended for character data), then each element of the array representing an existing value is encapsulated in `<e>` (or `<ce>` for complex numbers). For missing values, `<na/>` has to be used, empty values are just represented by `<e/></e>`.

The `type` attribute specifies the statistical data type, as logical, nominal, numeric, character and date/time. The optional `mode` attribute allows for further specification: nominal data could be unordered ("factors"), ordered and cyclic (e.g., days of week), whereas numeric data could be integer, real or complex.

As an example, consider a character dataset formed by color names, with one value missing (after green), and one being empty (after blue). The corresponding data section would appear as follows:

```
<data type="nominal" mode="unordered">
  <e>red</e> <e>green</e> <na/> <e>blue</e> <e></e> <e>yellow</e>
</data>
```

IEEE Number Format

The implementation is responsible for the correct casts. The number format has to follow the IEEE Standard for Binary Floating Point Arithmetic (see Institute of Electrical and Electronics Engineers, 1985), which is implemented by most programming languages and system libraries. However, the IEEE special values `+Inf`, `-Inf` and `NaN` must explicitly be specified by `<posinf/>`, `<neginf/>` and `<nan/>`, respectively, to facilitate the parsing process in case the IEEE standard were not implemented.

These special values could appear as follows:

```
<data type="numeric" mode="real">
  <e>1.23</e> <e><posinf/></e> <e><nan/></e> <e>2.43</e>
</data>
```

Complex Numbers

Complex numbers are enclosed in `<ce>` tags which contain exactly one `<r>` tag (for the real part) and one `<i>` tag (for the imaginary part). Apart from that, the same rules as for `<e>` apply:

```
<data type="numeric" mode="complex">
  <ce> <r>12.4</r> <i>1</i> </ce>
</data>
```

Date and Time Information

Data of type `datetime` has to follow the ISO 8601 specification (see International Organization for Standardization, 1997). StatDataML should only make use of the complete representation in extended format:

```
CCYY-MM-DDThh:mm:ss±hh:mm
```

For example, the 12th of March 2001 at 12 hours and 53 minutes, UTC+1, would be represented as: 2001-03-12T12:53:00+01:00.
3.5 Reference Implementations

Software is available for Matlab, Octave, Splus, R, Gnumeric; a conversion tool for SPSS is currently under development.

4 Conclusion

StatDataML seems general and flexible enough to cover most of statisticians’ data representation needs, although one might miss features like data inheritance and support for distributed data (e.g. via URLs or SQL queries on databases). The representation of high level objects (like time series) and statistical models are currently under investigation.

References


Institute of Electrical and Electronics Engineers (1985). IEEE Standard 754-1985 (R 1990), Standard for Binary Floating-Point Arithmetic.

