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Random XML sampling the Boltzmann way

Alexis Darrasse

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In this article we present the prototype of a framework capable of producing, with linear complexity, uniformly random XML documents with respect to a given RELAX NG grammar. The generation relies on powerful combinatorial methods together with numerical and symbolic resolution of polynomial systems.

1 Introduction

The Extensible Markup Language (XML) is extensively used today, either to encode documents (like in XHTML) or to serialize structured data. The XML standard[4] only defines some basic syntax rules followed by well-formed documents. However applications often define a set of higher order syntactic¹ rules that an XML document must respect to be considered as valid for the given application. A set of such rules is called a schema and is defined in one of several languages, like DTD, XML Schema, RELAX NG and others. We chose to deal with RELAX NG for its simplicity and solid theoretical basis.

Our work is based on the observation that RELAX NG[2] has essentially the same expressive power as the specifications of combinatorial structures using only union, product, sequence and allowing for recursive definitions. This means that valid XML documents are just trees and can be efficiently generated using a Boltzmann sampler[1].

In Boltzmann sampling we can easily derive a generator from the description of a combinatorial class. This generator has the following characteristics:

- it needs a precalculation that must be done once and involves finding a particular solution of a polynomial system,
- the sampling itself involves only basic mathematic operations and has a linear complexity in the size of the generated object and
- the size of the generated object is a random variable following a power law distribution.

We go from a RELAX NG grammar to a random XML document in three steps:

¹often called semantic

1. translating the grammar to a system of equations,
2. solving the system of equations and
3. sampling XML documents.

The first two steps need to be executed only once for a given grammar and their cost is only dependant on the complexity of the grammar. The final step has a complexity that is linear in the size of the result.

The current prototype includes a ruby program executing the first and last step and a maple program dealing with the second step. Future versions could consist of a single program not depending on a computer algebra system.

Even in its current form, our framework is capable of generating documents for all RELAX NG grammars that we were able to find, include XHTML, MathML, SVG, DocBook, OpenDocument and RELAX NG itself.

2 Translating the RELAX NG

We parse the RELAX NG document to get a combinatorial description of the grammar in the form of an Abstract Syntax Tree (AST). Every RELAX NG element is matched to a combinatorial construction, for example `choice` to union, `group` to product, `oneOrMore` to sequence etc.

The mapping from RELAX NG to combinatorial constructions is not unique, we thus have to make a few arbitrary decisions. First of all, we must decide of a way to count the size of an XML document, while satisfying the constraint that there must be a finite number of XML documents for a given size. Our choice is to count the number of elements plus the number of attributes.

Some facts on the AST: at the root we have the definition of `start` which is our entry point to the grammar and the definition of every `element` of the grammar. We can thus represent the AST as a forest, with every root being the definition of an `element`. `ref` elements found in different parts of the AST point to one of these definitions, which can lead us to see the AST also as a graph.

Note on data

Our framework concentrates on the tree-form structure of the XML document and treats `data` elements as simple leaves. These elements however represent data respecting arbitrarily complex datatypes which cannot be reasonably treated by a generic framework. We thus provide the possibility to call an arbitrary (written in Ruby since performed at step 3) function when the generator needs a value of a `data` element.

Even though the RELAX NG language does not provide a collection of basic datatypes, the XML Schema Datatypes[5] are used as such. We thus provide default samplers for each of the datatypes contained in this library, while preserving the possibility for the users to overload them.

Note on uniformity

One of the main advantages of using Boltzmann sampling is that it guarantees the uniformity of the distribution inside each size class. The simplifications made in our prototype break this uniformity in two ways:

- sets of attributes are considered as sequences, so `` and `` count as two different XML documents, while they are the same (but two attributes of the same element will always have different names) and
- the `interleave` element, which calls for the interleaving of it's arguments, is not taken into account, so all the interleavings count as a single element.

3 Solving the system of equations

The AST is fed to a Maple program that solves the set of equations defining the grammar and provides us with the constants needed for sampling. The calculation time needed for this operation depends heavily on the size and structure of the grammar. The user can use this Maple program as a black box, as it is not interactive. But for the purpose of explanation we now describe it a little more precisely.

A RELAX NG grammar defines, in our point of view, a (combinatorial) family of trees. As for every other combinatorial class, a generating function $C(x) = \sum_{n=0}^{\infty} t_n x^n$ is associated to this family, with t_n being the number of different trees of size n . An important parameter is the radius of convergence ρ of the generating function $C(x)$. The Boltzmann sampler uses the value of $C(x)$ and some related generating functions for a given parameter x . In the case of trees, ρ is an excellent choice for x [1].

The AST of the grammar can be directly translated into an algebraic system (that can itself be simplified to a polynomial one) defining the generating function $C(x)$. To be able to sample we need to solve two problems: evaluate the radius of convergence of the system and find its only solution that corresponds to C .

A major difficulty comes from the fact that simply solving the system for a given x gives us a set of solutions with no simple way of finding the good one. Thankfully, a combinatorial interpretation of Newton's method[3] gives us a very efficient and guaranteed numerical algorithm for evaluating $C(x)$.

As for the radius of convergence, for the time being, using a dichotomy approach and Newton algorithm we obtain an estimation. We can also (see section 5) take advantage of the particularities of the generating functions arising from grammars defining trees, in which the radius of convergence can be automatically calculated, as explained in [1].

To experiment the solving algorithm, we tried it on different RELAX NG grammars (found for most of them on the internet). Table 1 shows some measures on the grammars related to their complexity, together with the time needed

grammar	file	sing.	# el.	s.c.c.	newton	# eq.	# mon.	# sol.
ternary trees	1024	0.52912	2	1	0.260s	3	10	3
RSS	9.5K	0.44721	10	1	0.320s	16	79	2
PNML	23K	0.22526	22	1	0.322s	36	193	4
ILP 1	21K	0.23696	20	6	0.416s	27	211	9
ILP 6	99K	0.13951	51	31	0.828s	72	948	6
RELAX NG	124K	0.04127	33	18	0.696s	114	3725	32
XSLT	168K	0.05283	40	17	0.469s	122	1503	10
XHTML	289K	0.02456	47	32	0.932s	134	2077	26
XML Schema	237K	0.08615	59	9	0.528s	188	143465	
XHTML basic	284K	0.03039	53	38	1.080s	96	2073	13
XHTML strict	1.2M	0.01991	80	58	2.414s	151	6445	32
XHTML	1.5M	0.01609	93	66	3.798s	172	8449	56
SVG tiny	1.6M	0.03542	49	7	0.371s	101	4390	34
SVG full	6.3M	0.01834	118	27	0.718s	232	13831	
MathML	2.2M	0.00318	182	48	2.432s	265	265159	18
OpenDocument	2.8M	0.01757	500	101	6.544s	814	8890517	
DocBook	11M	0.01627	407	295	143.411s	977	183051	

Table 1: Evaluating the generating functions of different RELAX NG grammars. Measures made on a 3.2GHz Xeon with 6GB of RAM, using Maple 10 in a 64bit environment.

to evaluate the corresponding generating functions. The size of the corresponding polynomial systems is also mentioned, showing that solving them with a symbolic approach is a challenge. Here is a precise description of the column headers:

sing. Lower bound on the singularity of the system of equations.

file. Size of the file containing the grammar in Simple RELAX NG.

el. Number of **e**lement definitions.

s.c.c. Size of the biggest strongly connected component of the grammar.

newton Time needed to evaluate the values of the generating functions using the newton algorithm.

eq. Number of equations defining the polynomial system.

mon. Number of monomials in the polynomial system.

sol. Number of solutions of the zero-dimensional system, given a parameter smaller than the singularity.

These results show that with the numerical method we were able to deal with all the grammars in a very reasonable time.

4 Generating XML documents

To generate the XML documents the Boltzmann way, we explore the AST, starting from the **start** element of the grammar and treating the different elements the following way:

- for a union we choose randomly between the two siblings,
- for a product we take both children,
- for a sequence we take the child a random number of times,
- for a **ref** we continue at the corresponding **e**lement,
- for a leaf produce the corresponding value.

Thus the cost to produce an XML document is proportional to the size of the document and the constant factor depends on the grammar. That size however is random and actually follows a power law distribution. This means that we generate a very large number of very small documents and from time to time a huge document, eventually bigger than we can handle.

For this reason we include a mechanism for rejecting documents whose size falls outside a given window. The cost of the rejection can be precisely estimated[1]: generating a document of size $n(1 \pm \epsilon)$, for a fixed tolerance ϵ , costs $O(n)$, while generating a document of size exactly n costs $O(n^2)$ (costs are average, in the worst case the generator never returns a valid document, but this happens with probability zero).

5 Work in progress

The current state of our work shows what can be achieved by applying the Boltzmann sampling techniques in the problem of sampling random XML documents. We are in the process of completing and extending our framework in order to create tools useful as-is in a large number of use cases.

Efficient implementation and integration of the framework. The current implementation of our framework is a prototype with a design targeting flexibility and ease of development. Consequently it lacks in efficiency and ease of deployment, which will be the goals of future versions.

Progressive serialisation of the generated document. To be able to sample documents of millions of elements, or more, we can no longer keep the whole document in memory. The solution is to write the data on disk as soon as we know its position in the resulting document. This should be trivial for grammars not containing `interleave` constructions and could be reasonably treated even in that case.

Conserve the entropy, guarantee the precision. By implementing the non-deterministic parts of the samplers using bitwise comparisons, we can make sure not to use more entropy bits than necessary. At the same time we can check that the precision used for calculating the constants is sufficient, and if not, get more precision from the solver.

Assure uniformity in all cases. The bias introduced in the sampling by the simplified treatment of the `interleave` element and the attributes could be dealt with, if necessary. The set construction is already treated in the Boltzmann sampling, but leads to systems that are no longer polynomial. The treatment of the `interleave` construction is work in progress.

References

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