# The External Representation of Block Designs

Peter J. Cameron, Peter Dobcsányi, John P. Morgan, Leonard H. Soicher

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## 1 Introduction

This document should be of interest to those working in combinatorial or statistical design theory, as well as those interested in the development of standard electronic formats for mathematical objects.

We at *DesignTheory.org* are in the process of developing a web-based Design Theory Resource Server (DTRS) for combinatorial and statistical design theory. One critical element is our *External Representation of Designs* which will be used to store designs and their combinatorial, group theoretical and statistical properties in a standard platform-independent manner (*external* means external to any software). This will allow for the straightforward exchange of designs and their properties between various computer systems, including databases and web servers, and combinatorial, group theoretical and statistical packages. The external representation will also be used for outside submissions to our design database.

We have concentrated our initial development effort in the area of block designs, and in this document we present our standard for the *External Representation of Block Designs*. We shall give a full explanation and provide examples. We have tried to make the document readable by non-experts, since we don't expect everyone to be an expert in all the areas covered.

## 1.1 A Simple Example

We start with a simple example. It is a list of designs, in our external representation, containing a single design, known as the *Fano plane*.

The design is described in XML. Later in this document we discuss why we have chosen XML for the specification of block designs. For now, if you stare at the code, you will see that, at the first level of indentation, between the opening and closing tags **block\_design**, we have indeed specified the design: it has v = 7 points, b = 7 blocks, and the seven blocks are listed (the first one is [0, 1, 2], and there are tags to identify each of 0,1,2 as an integer). There is also a identification string for the design.

In XML, there are two ways of providing information, which we refer to as "attributes" and "elements". An "attribute", such as v, b or id, occurs within a tag, whereas an "element", such as blocks occurs within the scope of the tag. An XML document has the structure of a tree; the elements are the nodes of the tree, and the attributes are associated with nodes. We will use the general term "properties" in something like its mathematical sense, describing both attributes and elements.

This document contains our specification of an "external representation" of block designs, together with an explanation of the terms used, and some justification for doing it in the way we have chosen.

## 2 What is a Block Design?

Block designs are viewed in different ways by combinatorialists and statisticians. To a statistician, a block design is a set of "plots" or "experimental units" which carries a partition into "blocks", and a function from this set to the set of "treatments". A combinatorialist regards the set of treatments as basic (and usually calls them "points"), and identifies each block with the multiset of treatments occurring on plots in that block; thus, a block design is a set of points together with a multiset of multisets of points.

A multiset is essentially the same thing as a sorted list which may contain repeated items. In this documentation, we represent a multiset as a list in square brackets []. (The XML representation is a bit more complicated, as the above example shows.)

For the purpose of this specification, we have chosen to use the representation as a multiset of multisets.

Here is a small example. Suppose that we have six plots, numbered 1, 2, 3, 4, 5, 6, with blocks [1, 2, 3] and [4, 5, 6]. Suppose that treatment A is applied to plots 1, 2, 4, 5, and treatment B to plots 3 and 6. Then we represent the block design as having point set [A, B] and blocks [[A, A, B], [A, A, B]]. (Since the

lists are sorted, we would represent the design in same way even if, say, treatment B was applied to plots 1 and 5.) The names of the plots have disappeared, but the plots can be recovered as incident point-block pairs or "flags". We always represent block designs in this way.

In this example, blocks have the awkward property that they are multisets (rather than sets) of points. While this does occur in practice, we have decided to exclude such designs for the time being, for various reasons. A block design is called *binary* if no treatment occurs more than once in a block, that is, if the blocks are represented by sets (rather than general multisets) of points. All block designs in this document will be binary.

Here is an example of a binary design. It is the Fano plane from the Introduction, viewed in a slightly different way. There are 21 plots, partitioned into seven blocks of three; there are seven treatments, numbered from 0 to 6, as shown in the following table (whose columns represent the blocks):

0	0	0	1	1	2	2
1	3	5	3	4	3	4
2	4	6	5	6	6	5

Further details can be found in the items on block designs in the Encyclopaedia of Design Theory, or in our survey paper [1].

## 3 The Concept of External Representation

The concept of External Representation of designs can be best understood through its role in the operation of the Design Theory Resource Server (DTRS). DTRS has many faces, it will be an ever growing database of designs, application server, web server for design related online documents, software repository etc. The main purpose of the external representation is to provide a platform independent method for information exchange about designs. With other words, the external representation acts as a *communication protocol* specialized for "talking about designs". This protocol is used in communication between various components of DTRS and its users. Here the concept "users" covers both human and software agents. Some examples for such communicating agents: database back-end for storing designs, middle layers between the database and the web and/or application servers, a researcher uploading some particular collection of designs, a user searching for designs having given properties, a statistical application program directly accessing the DTRS database etc. While these agents are free to use any internal representation of designs, they must use the standard external representation when they communicate with each other.

The external representation is used in three main areas:

- 1. An external representation is a formalism to encode various classes of designs as mathematical objects together with their most important properties. Many of these properties are complex mathematical objects in their own right.
- 2. The external representation can define invariants of a given list of designs. The use of such invariants provides a method for formulating complex queries about designs. A query will be expressed in terms of list invariants and the reply to this query will be a list of designs satisfying these invariants.
- 3. The external representation will be used as a specification tool to determine the content and, to some extent, the structure of the DTRS design database. Note, however, the database's internal representation can (and probably will) be quite different from this format.

Based on the above functionalities, we have determined the main technical requirements for an external representation as it follows.

- It can express the particular mathematical structures.
- It represents a hierarchical structure: a rooted, labelled tree.
- It is hardware/software platform independent and text based.
- It can be easily parsed.

Satisfying the requirements outlined above, one can think of many different implementations fitting the bill. We mention here two possibilities: the oldest, Lisp S-expressions; and the recently most popular, XML. Out of practical considerations, we have decided to use XML.

This document specifies an XML based implementation of the external representation for block designs. We focus mainly on the first area listed above, that is encoding block designs and their properties. The other two functionalities and other types of designs are subjects of further research and development.

We use the Relax NG [6] schema language for XML in *compact syntax* to specify the external representation. The reader can find the complete schema in Appendix A. It is also available as a separate file design.rnc for the purpose of direct computer use.

## 4 Indexing and Functions

We describe here some conventions referring to the indexing of objects, and the representation of functions.

## 4.1 Indexing and Ordering

We adopt the convention that, if a block design has v points, then the points are the integers  $0, 1, \ldots, v - 1$ . This is a combination of two assumptions: the points are ordered; and the index set starts at 0 (rather than 1).

There are several choices of ordering of sets (or multisets) of points. We have chosen to order in the following way:

- first compare the length of the two lists; the shorter comes first.
- for lists of the same length, we order lexicographically. (Recall that the lists are sorted.)

So for example, here are a few sets in order:

[2], [0, 1], [0, 2], [1, 2], [1, 2], [0, 1, 3], [1, 2, 3], [0, 1, 2, 3]

For the purpose of defining functions on the collection of blocks, we now index these blocks from 0 to b - 1, where b is the number of blocks of the design. If the above list contains all the blocks of a certain design D, then we can refer to block 5 of D, which will be the set [0, 1, 3] in this case.

The same principle can be extended to lists of lists. Assuming that the "inner" lists are already ordered, we first compare the length of the two lists,

and if they are equal, we order the lists "lexicographically" (with the order previously defined between list elements). This process can be continued recursively to any level of nesting.

However, we do not require that this ordering is adhered to throughout the tree. The following objects may be required to be ordered (they have a boolean attribute ordered):

- blocks
- function\_on\_indices
- function\_on\_ksubsets\_of\_indices
- cycle\_type

Functions on indices, and on k-subsets of indices, are described next. For cycle types, see the section 7.4 on Automorphisms.

## 4.2 Functions and Index Flags

A function f with finite domain can be given by listing all (x, f(x)) pairs. Note that this list when spelled out in XML format can be a very large one, in particular, if the x-s are complex objects on their own. To help on this problem we can do several things:

• Instead of using *x*-s themself we use only indices referring to them. function\_on\_indices is defined to do this.

The underlying principle is that if the external representation explicitly contains the related objects in a well defined (canonical) order then, in general, we use indexing as a way to refer to these objects. Nesting, in this sense, is not allowed.

- Frequently the domain of our functions is the set of *k*-subsets of some of our objects. function\_on\_ksubsets\_of\_indices is defined for this situation.
- Regarding the (x, f(x)) pair, we allow several kinds of "contractions" (see map below):

- If different x-s map to the same image, then instead of listing all these pairs we say  $(\{x, x_1, x_2, \ldots\}, f(x))$ . If the function f has just one image f(x) we may say (entire\_domain, f(x)).
- Sometimes the user is not interested in the preimage  $\{x, x_1, x_2, \ldots\}$ of f(x), but only in its cardinality, so we allow  $(|\{x, x_1, x_2, \ldots\}|, f(x))$ .
- Finally, we even allow leaving the preimage part of the pair blank, just giving the list of function values (f(x)).

In fact, the user may only be interested in the image cardinality, in which case the entire function body may be blank.

In more detail:

```
function_on_indices = element function_on_indices {
    attribute domain { "points" | "blocks" } ,
    attribute n { xsd:nonNegativeInteger } ,
    attribute ordered { "true" | "unknown" } ,
    attribute image_cardinality { xsd:positiveInteger } ? ,
    attribute precision { xsd:positiveInteger } ? ,
    attribute title { text } ? ,
    ( map + | blank )
}
```

This specifies a function on either points or blocks. **n** is the cardinality of the domain. **ordered** specifies whether the function entries are ordered (by preimages): if the function body is not blank and each preimage is given explicitly or (if there is just one function image) as the empty element **entire\_domain** (i.e. neither as a **preimage\_cardinality** nor **blank**), then the value of ordered must be "true", otherwise it is "unknown". **precision** is required if the function values are real numbers and specifies the precision to which they have been computed. A function is given by a sequence of **map**'s, each of which is specified as follows:

```
map = element map {
   ( preimage | preimage_cardinality | blank )
   ,
   element image { z | d | q | not_applicable }
}
preimage = element preimage {
```

```
z +
|
element ksubset { z+ } +
|
entire_domain
}
```

```
preimage_cardinality = element preimage_cardinality { z }
```

For an example of the use of function\_on\_indices, see section 7.5 on Resolutions.

The function\_on\_ksubsets\_of\_indices specification works in the same way when the domain consists of all sets of points or blocks of fixed size k:

```
function_on_ksubsets_of_indices = element function_on_ksubsets_of_indices {
    attribute domain_base { "points" | "blocks" } ,
    attribute n { xsd:nonNegativeInteger } ,
    attribute k { xsd:nonNegativeInteger } ,
    attribute ordered { "true" | "unknown" } ,
    attribute image_cardinality { xsd:positiveInteger } ? ,
    attribute precision { xsd:positiveInteger } ? ,
    attribute title { text } ? ,
    ( map + | blank )
}
```

For an example of its use, see the section 7.3.1 on Point concurrences.

We use the concept of index\_flag to store an element in a list of "fuzzy booleans":

```
index_flag = element index_flag {
    attribute index { xsd:nonNegativeInteger },
    attribute flag { "true" | "false" | "unknown" }
}
```

For example, we may want to record for which values of  $\alpha$  a design is  $\alpha$ -resolvable; for each value of  $\alpha$ , the answer may be "true", "false", or "un-known".

## 5 Permutation groups

Permutation groups appear in many areas of design theory, in particular as automorphism groups of designs.

The specification of an permutation group is:

```
permutation_group = element permutation_group {
   attribute degree { xsd:positiveInteger } ,
   attribute order { xsd:positiveInteger } ,
   attribute domain { "points" },
   generators ,
   permutation_group_properties?
}
```

There are four compulsory properties:

#### degree

An attribute giving the number n of points on which the permutations are defined (the permutation group will then act on the indices  $\{0, \ldots, n-1\}$ ).

#### order

An attribute giving the number of permutations in the group.

domain An attribute specifying the domain indexed by the points  $0, \ldots, n-1$ .

#### generators

A list of permutations which generate the group. A permutation is represented by the ordered list of its values (the images of the points  $0, \ldots, n-1$  under the permutation).

For example, the permutation group which is the automorphism group of our Fano plane can be given as:

```
<permutation_group degree="7" domain="points" order="168">
    <generators>
        <permutation>
            <z>1</z>
            <z>0</z>
```

<z>2</z> <z>3</z> <z>5</z> <z>4</z> <z>6</z> </permutation> <permutation> <z>0</z> <z>2</z> <z>1</z> <z>3</z> <z>4</z> <z>6</z> <z>5</z> </permutation> <permutation> <z>0</z> <z>3</z> <z>4</z> <z>1</z> <z>2</z> <z>5</z> <z>6</z> </permutation> <permutation> <z>0</z> <z>1</z> <z>2</z> <z>5</z> <z>6</z> <z>3</z> <z>4</z> </permutation> <permutation> <z>0</z> <z>1</z> <z>2</z> <z>4</z> <z>3</z> <z>6</z> <z>5</z> </permutation> </generators> </permutation\_group>

There are also various properties which can optionally be specified:

#### primitive

True if the group acts primitively on points. A permutation group is *primitive* if it preserves no non-trivial equivalence relation. By convention, we assume that a primitive group is transitive (that is, any point can be carried to any other by some group element). (So the trivial group acting on two points is not primitive.)

## generously\_transitive, multiplicity\_free, stratifiable

Each orbit of the group acting on the set of ordered pairs of points can be represented by a matrix of zeros and ones of order n (which can be thought of as the characteristic function of the orbit). These basis matrices span the centraliser algebra of the group (the algebra of all matrices commuting with the group elements). Now the group is generously transitive if all the basis matrices are symmetric; it is multiplicity-free if the basis matrices commute; and it is stratifiable if the symmetrised basis matrices commute. Each concept implies its successor in the order given.

A transitive permutation group is generously transitive iff any two points can be interchanged by some element of the group; it is multiplicityfree iff no irreducible constituent of the permutation character occurs with multiplicity greater than 1; and it is stratifiable iff the orbits of the group on unordered pairs form an association scheme. All these properties are false if the group is not transitive.

### no\_orbits

The number of orbits on points. The group is transitive exactly when there is just one orbit on points.

### degree\_transitivity

The maximum number s such that the group is s-transitive on points (that is, any s-tuple of distinct points can be carried to any other by some group element).

## rank

The number of orbits of the group on the set of ordered pairs of points. Note that this is defined for any permutation group; if the group is transitive, it is equal to the number of orbits of the stabiliser of a point.

```
cycle_type_representatives
see below
```

The cycle type of a permutation is the multiset of its cycle lengths (when it is written as a product of disjoint cycles). The element cycle\_type\_representative consists of a cycle type and an element of the group having that cycle type, and optionally the number of elements of the group having that cycle type. cycle\_type\_representatives is a list of these cycle\_type\_representative elements, one for each cycle type represented by an element of the group.

For the example above, there are five cycle types, [7], [1, 2, 4], [1, 3, 3], [1, 1, 1, 2, 2], and [1, 1, 1, 1, 1, 1] (the last being the identity). The cycle type representative for the second type is:

```
<cycle_type_representative>
<permutation>
<z>0</z>
<z>2</z>
<z>1</z>
<z>5</z>
<z>5</z>
<z>6</z>
<z>4</z>
<z>3</z>
</permutation>
<cycle_type ordered="true"><z>1</z><z>2</z><</cycle_type>
<no_having_cycle_type>
<z>42</z>
</no_having_cycle_type>
</cycle_type_representative>
```

## 6 Numerical Data Types

Some of the numerical data in the external representation are the result of possibly inexact computations. Basically, there are three sources of this inaccuracy:

- The inaccuracy of the finite floating point representation.
- Arithmetical errors during computation.
- Cutting short an otherwise infinite approximation process.

The end result is that, in general, numbers in the external representation can be considered correct only within certain limits. We say they are "precise" up to some significant figures (see the details below).

The external representation version 1.1 provides the following *numerical data types*:

- Arbitrary precision *integers* (element <z>).
- Arbitrary precision *rationals* (element <q>) written in *a/b* format where *a* and *b* are integers.
- Floating point *decimals* (element <d>) up to some given precision specified as the number of significant digits.

A conforming software implementation must provide the corresponding internal representations.

Here are the rules for representing numerical data in the external representation:

- If a number is the result of an inexact computation then it must be represented using the *decimal data type*.
- The decimal representation of an inexact number must always contain the decimal point regardless the number would round up to an integer.
- Exact numbers must be represented either using the *integer* or the *rational data type*.

The precision of decimal numbers is indicated by an optional attribute precision of particular elements. The elements which can have this attribute are: <list\_of\_designs>, <block\_design>, <function\_on\_...>, <statistical\_properties>. The rationale for having many elements with the optional precision attribute is to provide flexible scoping rules and avoid unnecessary repetition.

The **precision** attribute gives the *number of significant figures* of all decimal numbers in the tree whose root contains the attribute. This precision can be overridden by giving different precision in one or more subtrees. In general, a precision of a decimal number is the precision given in the root of the smallest subtree containing the number and with a root having a specified precision attribute. If an external representation document contains any data which is the result result of inexact computation, precision must be specified.

## 7 Block Designs

Recall our blanket assumption that all block designs are *binary*: this means that no treatment occurs more than once in a block, so that the blocks are sets rather than general multisets. However, it can happen that the same set occurs more than once in the list of blocks; that is, the list of blocks may be a multiset. In this case we say that the design has *repeated blocks*.

## 7.1 Essential Properties

The specification of block\_design is as follows:

```
block_design = element block_design {
    attribute id { xsd:ID } ,
    attribute v { xsd:positiveInteger } ,
    attribute b { xsd:positiveInteger } ? ,
    attribute precision { xsd:positiveInteger } ? ,
    blocks ,
    point_labels ? ,
    indicators ? ,
    combinatorial_properties ? ,
    block_design_automorphism_group ? ,
    resolutions ? ,
    statistical_properties ? ,
    alternative_representations ? ,
    info ?
}
```

The first four components of the specification are:

id

An attribute giving a unique identifier for the design.

v

An attribute giving the number of points.

b

An attribute giving the number of blocks (optional).

### blocks

The list of blocks (as described above). The list must be ordered:

```
blocks = element blocks {
    attribute ordered { "true" } ,
    block+
}
block = element block { z+ }
```

Here is the design from the example in the Introduction, including only the components above:

```
<block_design b="7" id="t2-v7-k3-L1-1" v="7">
        <blocks ordered="true">
            <block><z>0</z><z>1</z><z>2</z></block>
        <block><z>0</z><z>3</z><z>4</z></block>
        <block><z>0</z><z>3</z><z>4</z></block>
        <block><z>0</z><z>3</z><z>4</z></block>
        <block><z>0</z><z>3</z><z>4</z></block>
        <block><z>0</z><z>3</z><z>6</z></block>
        <block><z>1</z><z>3</z><z>6</z></block>
        <block><z>1</z><z>3</z><z>6</z></block>
        <block><z>2</z><z>4</z><z>6</z></block>
        <block><z>2</z><z>4</z><z>6</z></block>
        <block><z>2</z><z>4</z><z>6</z></block>
        <block><z>2</z><z>4</z><z>6</z></block>
        <block><z>2</z><z>4</z><z>6</z></block>
        <block><z>2</z><z>4</z><z>6</z></block>
        <block><z>2</z><z>4</z><z>6</z></block>
        <block><z>2</z><z>4</z><z>6</z></block>
        <block><z>2</z><z>4</z><z>6</z></block>
        <block><<z>6</block></block></block>
        <block><z>2</z><z>4</z><z>6</z></block>
        <block><z>2</z><z>4</z><z>6</z></block>
        <block><z>2</z><z>4</z><z>6</z></block>
        <block><z>2</z></block>
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```

All these components, except the attribute **b**, are essential. The subsequent elements are optional. The first optional element is point\_labels. If, for example, the design has been built from a set of points in a projective geometry, the point labels might be the coordinates of the points. More important for applications, the point labels could be the actual treatments associated to the points in the experimental plan (after randomisation). The point labels, if present, should form a list of length v.

## 7.2 Indicators

Indicators are boolean variables which record certain properties which a block design may have. We have included the following indicators:

#### repeated\_blocks

True if the same set occurs more than once in the list of blocks.

## resolvable

True if the design has a *resolution*, which is a partition of the blocks into subsets called *parallel classes* or *resolution classes*, each of which forms a partition of the point set.

### affine\_resolvable

True if the design is *affine resolvable*, which means that the design is resolvable and any two blocks not in the same parallel class of a resolution meet in a constant number  $\mu$  of points. If the design is affine resolvable then we optionally give this constant  $\mu$  (unless the design consists of a single parallel class, in which case  $\mu$  is not defined).

#### equireplicate

True if each point lies in a fixed number r of blocks. If so, then we also optionally give the replication number r.

#### constant\_blocksize

True if each block contains a fixed number k of points. If so, then we optionally also give the block size k.

#### t\_design

True if the block design is a t-design for some t > 1. This means that the design has constant block size and that any t points are contained in a positive constant number  $\lambda$  of blocks. If so, then we optionally give the maximum value of t for which this holds.

#### connected

True if the incidence graph of the block design is a connected graph. (The *incidence graph* or *Levi graph* of a block design is the bipartite graph whose vertices are the points and blocks of the design, a point and block being adjacent if the point is contained in the block.) We optionally give the number of connected components of the incidence graph.

#### pairwise\_balanced

True if v > 1 and the number of blocks containing two distinct points is a positive constant  $\lambda$ . If so, then we optionally give this  $\lambda$ .

## variance\_balanced

True if v > 1 and the intra-block information matrix has v-1 identical,

nonzero eigenvalues. Equivalently, the v - 1 canonical variances are all equal (and finite). For definitions of terms used here, see section 7.6 on Statistical Properties.

## efficiency\_balanced

True if v > 1 and the v - 1 statistical canonical efficiency factors are identical and nonzero. For equireplicate designs, this is equivalent to variance\_balanced, but not genenerally otherwise. Also see the section 7.6 Statistical Properties.

#### cyclic

True if the design has an automorphism which permutes all the points in a single cycle.

### one\_rotational

True if the design has an automorphism which fixes one point and permutes the other v - 1 points in a single cycle.

In the last two cases, an automorphism with the stated properties can be found under cycle\_type\_representatives, described in section 7.4 on Automorphisms.

The several different sorts of balance are explained in the Encyclopaedia. For a (binary) design with constant block size, variance balance reduces to pairwise balance. For a equireplicate (binary) design with constant block size, efficiency balance reduces to pairwise balance.

The indicators for our example are:

#### <indicators>

```
<repeated_blocks flag="false">
</repeated_blocks>
<resolvable flag="false">
</resolvable>
<affine_resolvable flag="false">
</affine_resolvable>
<equireplicate flag="true" r="3">
</equireplicate flag="true" r="3">
</equireplicate flag="true" r="3">
</constant_blocksize flag="true" k="3">
</constant_blocksize>
<t_design flag="true" maximum_t="2">
</t_design>
<connected flag="true" no_components="1">>
```

```
</connected>
<pairwise_balanced flag="true" lambda="1">
</pairwise_balanced>
<variance_balanced flag="true">
</variance_balanced flag="true">
</efficiency_balanced>
<cefficiency_balanced</p>
</efficiency_balanced>
<cyclic flag="true">
</cyclic>
<one_rotational flag="false">
</one_rotational>
</indicators>
```

## 7.3 Combinatorial Properties

Combinatorial properties are those which can be computed exactly from the list of blocks of the design. We include the following:

```
combinatorial_properties = element combinatorial_properties {
   point_concurrences ? ,
   block_concurrences ? ,
   t_design_properties ? ,
   alpha_resolvable ? ,
   t_wise_balanced ?
}
```

## 7.3.1 Point Concurrences

Each entry in the point\_concurrences is a function on the *t*-element sets of points, for some positive integer *t*, giving the number of blocks containing each *t*-set. We use the general mechanism for function\_on\_ksubsets\_of\_indices with k = t, to do this. Note that a block design is *t*-wise balanced (see 7.3.5) if and only if the point concurrence function for k = t takes only a single value.

For example, here is a small block design:

```
<block><z>1</z><z>2</z></block>
<block><z>0</z><z>1</z><z>2</z></block>
</blocks>
</block_design>
```

```
and here are its t-wise point concurrences for t = 1, 2:
<point_concurrences>
    <function_on_ksubsets_of_indices domain_base="points" k="1" n="3"
     ordered="true" title="replication_numbers">
        <map>
            <preimage>
                <entire_domain>
                </entire_domain>
            </preimage>
            <image><z>3</z></image>
        </map>
    </function_on_ksubsets_of_indices>
    <function_on_ksubsets_of_indices domain_base="points" k="2" n="3"
     ordered="true" title="pairwise_point_concurrences">
        <map>
            <preimage>
                <ksubset><z>0</z><z>2</z></ksubset>
            </preimage>
            <image><z>1</z></image>
        </map>
        <map>
            <preimage>
                <ksubset><z>0</z><z>1</z></ksubset>
                <ksubset><z>1</z><z>2</z></ksubset>
            </preimage>
            <image><z>2</z></image>
        </map>
    </function_on_ksubsets_of_indices>
</point_concurrences>
```

## 7.3.2 Block concurrences

Similarly, here we record the functions giving the numbers of points in the intersection of *t*-sets of blocks. The blocks are indexed from 0 to b-1, and we again use the general mechanism for function\_on\_ksubsets\_of\_indices.

In practice, we almost always use the compressed representation of this function where we give only the preimage cardinalities (as described in section 4.2 on Functions and index flags).

For example, in the Fano plane, any block contains three points, and any two blocks meet in one point. This is recorded as follows:

```
<block_concurrences>
    <function_on_ksubsets_of_indices domain_base="blocks" k="1" n="7"
     ordered="unknown" title="block_sizes">
        <map>
            <preimage_cardinality><z>7</z></preimage_cardinality></preimage_cardinality>
            <image><z>3</z></image>
        </map>
    </function_on_ksubsets_of_indices>
    <function_on_ksubsets_of_indices domain_base="blocks" k="2" n="7"
     ordered="unknown" title="pairwise_block_intersection_sizes">
        <map>
            <preimage_cardinality><z>21</z></preimage_cardinality>
            <image><z>1</z></image>
        </map>
    </function_on_ksubsets_of_indices>
</block_concurrences>
```

## 7.3.3 *t*-design properties

```
(To be extended)
```

This is the area of greatest interest to combinatorialists.

Let  $t, v, k, \lambda$  be natural numbers with  $t \leq k \leq v$  and  $\lambda > 0$ . A t- $(v, k, \lambda)$  design is a block design with the properties

- there are v points;
- each block contains exactly k points;
- any t points are contained in exactly  $\lambda$  blocks.

A *t*-design is a block design which is a t- $(v, k, \lambda)$  design for some  $v, k, \lambda$ .

If our design is a *t*-design for some t > 1, we record in the element t\_design\_properties the attributes  $t, v, b, r, k, \lambda$ . Here v and b have their usual meaning, r and k

are the replication number and block size, and t and  $\lambda$  have the properties of the definition. We do not guarantee that the design is not a t'-design for some t' > t. (On the other hand, a t-design is also an s-design for any s < t.)

We also record some properties of the t-design. At present, we have the following:

## square

True if the numbers of points and blocks are equal.

```
projective_plane
```

True if the design is a projective plane.

```
affine_plane
```

True if the design is an affine plane.

```
steiner_system
```

True if the design is a t-(v, k, 1) design for some t, v, k. We also record the relevant value of t (which may not be the same as the attribute called t).

```
steiner_triple_system
```

True if the design is a 2 - (v, 3, 1) design.

For example, the *t*-design properties of the Fano plane are as follows:

```
<t_design_properties>
<parameters b="7" k="3" lambda="1" r="3" t="2" v="7">
</parameters>
<square flag="true">
</square>
<projective_plane flag="true">
</projective_plane flag="true">
</projective_plane>
<affine_plane flag="false">
</affine_plane flag="false">
</steiner_system flag="true" t="2">
</steiner_system>
<steiner_triple_system flag="true">
</steiner_triple_system flag="true">
</steiner_triple_system>
</t_design_properties>
```

More properties will be included here. Among others, these will include different specific types of t-designs, and intersection triangles for Steiner systems.

## 7.3.4 $\alpha$ -resolvability

A resolution was defined above, but it can be described as a partition of the block multiset of the design into subdesigns, each of which is equireplicate with r = 1. More generally, an  $\alpha$ -resolution is a partition of the design into subdesigns, each of which is equireplicate with  $r = \alpha$ .

The element alpha\_resolvable is a list of index\_flags, which record, for relevant positive values of  $\alpha$ , whether the property is true, false or unknown.

```
alpha_resolvable = element alpha_resolvable {
    index_flag +
}
```

### 7.3.5 *t*-wise balance

A block design is *t*-wise balanced if each set of *t* distinct points is contained in a constant number of blocks; it does not imply constant block size. (The two properties together specify a *t*-design.) Unlike for *t*-designs, a block design may be *t*-wise balanced but not *s*-wise balanced for s < t. We store information about the values of *t* for which the design is *t*-wise balanced as list of index\_flags.

Here is an example of the t\_wise\_balanced element for the Fano plane:

```
<t_wise_balanced>
    <index_flag flag="true" index="1">
    </index_flag>
    <index_flag flag="true" index="2">
    </index_flag>
</t_wise_balanced>
```

## 7.4 Automorphisms

An *automorphism* of a block design is a permutation of the set of points of the design such that, if this permutation is applied to the elements of each block, the multiset of blocks is the same as before. (In other words: the block multiset is a list of lists; if we apply the permutation to all elements of the inner lists, re-sort each inner list, and then re-sort the outer list, the result is the same as the original list.) The collection of all automorphisms forms a *group*, that is, it is closed under composition of permutations. Thus, the automorphism group of a design is a permutation group on the set of points.

If the block design does not have repeated blocks, then each automorphism induces a permutation on the set  $[0, \ldots, b-1]$  of block indices: this permutation carries *i* to *j* if the image of the *i*-th block under the automorphism is the *j*-th block. In this case, the automorphism group has an induced action on the set of block indices. If there are repeated blocks, the action on the set of block indices is undefined.

For example, the example in the Introduction has an automorphism [1, 3, 5, 2, 0, 6, 4] (mapping 0 to 1, 1 to 3, etc.) Altogether this famous design has 168 automorphisms.

The specifications for automorphism groups and their properties for block designs are:

```
block_design_automorphism_group = element automorphism_group {
    permutation_group,
    block_design_automorphism_group_properties ?
}
block_design_automorphism_group_properties = element automorphism_group_properties {
    element block_primitive {
        attribute flag { "true" | "false" | "not_applicable" }
    } ?
,
    element no_block_orbits {
        attribute value { xsd:positiveInteger | "not_applicable" }
    } ?
,
    element degree_block_transitivity {
        attribute value { xsd:nonNegativeInteger | "not_applicable" }
    } ?
}
```

Permutation groups and their properties have already been described in section 5. Some properties of the automorphism group are specific to block designs, and are (optionally) described separately under automorphism\_group\_properties. They are: block\_primitive

True if the group acts primitively on blocks. (If there are repeated blocks, this is not defined, and takes the value not\_applicable.)

no\_block\_orbits

The number of orbits on blocks. (If there are repeated blocks, this is not defined, and takes the value not\_applicable.)

degree\_block\_transitivity

The maximum number s such that the group is s-transitive on blocks. (If there are repeated blocks, this is not defined, and takes the value not\_applicable.)

## 7.5 Resolutions

Recall that a *resolution* of a block design is a partition of the blocks into subsets, each of which forms a partition of the point set. Such a partition of the block (multi)set can be represented as a function on the set of indices of blocks (the parts of the partition being the preimages of the elements in the range of the function). We thus store a resolution as a function\_on\_indices with domain="blocks".

An *automorphism* of a resolution is a permutation of the set of points of the design such that, if this permutation is applied to the elements of each block in each resolution class, the (multi)set of resolution classes is the same as before. The collection of all automorphisms of a resolution of a design forms a subgroup of the automorphism group of the design itself, and we use the same **automorphism\_group** structure for the automorphism group of a resolution as we do for the automorphism group of a block design (although the **automorphism\_group\_properties** for a resolution are different than those for a block design).

We specify a resolution as follows:

```
resolution = element resolution {
   function_on_indices,
   resolution_automorphism_group ?
}
```

A block design D may have more than one resolution. We say that two resolutions R and S of D are *isomorphic* if there is an element g in the automorphism group of D, such that, when g is applied to the elements of each block in each resolution class of R, the resulting resolution is equal to S. Isomorphism defines an equivalence relation on the set of resolutions of D.

We use the element **resolutions** to store a nonempty list of (distinct) resolutions of a resolvable design. The attributes of this tag are used to specify whether the listed resolutions are pairwise nonisomorphic and whether all isomorphism classes of resolutions are represented in the list.

```
resolutions = element resolutions {
    attribute pairwise_nonisomorphic { "true" | "false" | "unknown" },
    attribute all_classes_represented { "true" | "false" | "unknown" },
    resolution +
}
```

We now display a famous resolvable design, the affine plane of order 3, which has just one resolution.

```
<list_of_designs design_type="block_design" dtrs_protocol="1.1" no_designs="1"</pre>
pairwise_nonisomorphic="true" xmlns="http://designtheory.org/xml-namespace">
    <block_design b="12" id="t2-v9-k3-L1-1" v="9">
        <blocks ordered="true">
            <block><z>0</z><z>1</z><z>2</z></block>
            <block><z>0</z><z>3</z><z>4</z></block>
            <block><z>0</z><z>5</z><z>6</z></block>
            <block><z>0</z><z>7</z><z>8</z></block>
            <block><z>1</z><z>3</z><z>5</z></block>
            <block><z>1</z><z>4</z><z>7</z></block>
            <block><z>1</z><z>6</z><z>8</z></block>
            <block><z>2</z><z>3</z><z>8</z></block>
            <block><z>2</z><z>4</z><z>6</z></block>
            <block><z>2</z><z>5</z><z>7</z></block>
            <block><z>3</z><z>6</z><z>7</z></block>
            <block><z>4</z><z>5</z><z>8</z></block>
        </blocks>
        <resolutions all_classes_represented="true"
         pairwise_nonisomorphic="true">
            <resolution>
                <function_on_indices domain="blocks" n="12" ordered="true"
                 title="resolution">
                    <map>
                        <preimage><z>0</z><z>10</z><z>11</z></preimage>
```

```
<image><z>0</z></image>
                        </map>
                        <map>
                             <preimage><z>1</z><z>6</z><z>9</z></preimage>
                             <image><z>1</z></image>
                        </map>
                        <map>
                             <preimage><z>2</z><z>5</z><z>7</z></preimage></preimage></preimage></preimage></preimage></preimage></preimage>
                             <image><z>2</z></image>
                        </map>
                        <map>
                             <preimage><z>3</z><z>4</z><z>8</z></preimage>
                             <image><z>3</z></image>
                        </map>
                   </function_on_indices>
              </resolution>
         </resolutions>
     </block_design>
</list_of_designs>
```

## 7.6 Statistical Properties

For a statistician, a block design is a plan for an experiment. The v points of the block design are usually called *treatments*, a general terminology encompassing any set of v distinct experimental conditions of interest. The purpose of the experiment is to compare the treatments in terms of the magnitudes of change they induce in a response variable, call it y. These magnitudes are called *treatment effects*.

In a typical experiment (there are many variations on this, but we stick to the basics to start), each treatment is employed for the same number rof experimental runs. Each run is the application of the treatment to an individual experimental unit (also called *plot*) followed by the observation of the response y. An experiment to compare v treatments using r runs (or "replicates") requires a total of vr experimental units.

If the vr experimental units are *homogeneous* (for the purposes of the experiment, essentially undifferentiable) then the assignment of the v treatments, each to r units, is made completely at random. Upon completion of the experiment, differences in treatment effects are assessed via differences in the v means of the observed values y for the v treatments (each mean is the average of r observations). This simplest of experiments is said to follow a *completely randomized design* (it is *not* a block design).

The concept of a *blocked* experiment comes into play when the vr experimental units are *not* homogeneous. A *block* is just a subset of the experimental units which are essentially undifferentiable, just as described in the previous paragraph. If we can partition our vr heterogeneous units into b sets (blocks) of k homogeneous units each, then after completion of the experiment, when the statistical analysis of results is performed, we are able to isolate the variability in response due to this systematic unit heterogeneity.

To make clear the essential issue here, consider a simple example. We have v = 3 fertilizer cocktails (the treatments) and will compare them in a preliminary greenhouse experiment employing vr = 6 potted tobacco plants (the experimental units). If the pots are identically prepared with a common soil source and each receiving a single plant from the same seed set and of similar size and age, then we deem the units homogeneous. Simply randomly choose two pots for the application of each cocktail. This is a completely randomized design. At the end of the experimental period (two months, say) we measure y = the total biomass per pot.

Now suppose three of the plants are clearly larger than the remaining three. The statistically "good" design is also the intuitively appealing one: make separate random assignments of the three cocktails to the three larger plants, and to the three smaller plants, so that each cocktail is used once with a plant of each size. We have blocked (by size) the 6 units into two homogeneous sets of 3 units each, then randomly assigned treatments within blocks. Notice that there are  $3! \times 3! = 36$  possible assignments here; above there were 6! = 720 possible assignments. Because k = v this is called a *complete* block design.

The statistical use of the term "block design" should now be clear: a block design is a plan for an experiment in which the experimental units have been partitioned into homogeneous sets, telling us which treatment each experimental unit receives. The external representation is a bit less specific: each block of a block design in external representation format tells us a set of treatments to use on a homogeneous set (block) of experimental units but without specifying the exact treatment-to-unit map within the block. The latter is usually left to random assignment, and moreover, does not affect the standard measures of "goodness" of a design (does not affect the information matrix; see below), so will not be mentioned again.

There are solid mathematical justifications for why the complete block design in the example above is deemed "good," which we develop next. This development does not require that k = v, nor that the block sizes are all the same, nor that each treatment is assigned to the same number of units. However, it does assume that the block sizes are known, fixed constants, as determined by the collection (of fixed size) of experimental units at hand. Given the division of units into blocks, we seek an assignment of treatments to units, i.e. a block design, that optimizes the precision of our estimates for treatment effects. From this perspective, two different designs are comparable if and only if they have the same v, b, and block sizes (more precisely, block size distribution).

Statistical estimation takes place in the context of a model for the observations y. Let  $y_{ij}$  denote the observation on unit i in block j. Of course we must decide what treatment is to be placed on that unit - this is the design decision. Denote the assigned treatment by d[i, j]. Then the standard statistical model for the block design (there are many variations, but here this fundamental, widely applicable block design model is the only one considered) is

$$y_{ij} = \mu + \tau_{d[i,j]} + \beta_j + e_{ij}$$

where  $\tau$  is the treatment effect mentioned earlier,  $\beta_j$  is the effect of the block (reflecting how this homogeneous set of units differs from other sets),  $\mu$  is an average response (the treatment and block effects may be thought of as deviations from this average), and  $e_{ij}$  is a random error term reflecting variability among homogeneous units, measurement error, and indeed whatever forces that play a role in making no experimental run perfectly repeatable. In this model the  $e_{ij}$ 's have independent probability distributions with common mean 0 and common (unknown) variance  $\sigma^2$ .

With n the total number of experimental units in a block design, the design map d (note: symbol d is used both for the map and the block design itself) from plots to treatments can be represented as an  $n \times v$  incidence matrix, denoted  $A_d$ . Also let  $N_d$  be the  $v \times b$  treatment/block incidence matrix, let K be the diagonal matrix of block sizes (= kI for equisized blocks), and write

$$C_d = A'_d A_d - N_d K^{-1} N'_d$$

which is called the *information matrix* for design d (note: A' denotes the transpose of a matrix A). Why this name? Estimation focuses on comparing the treatment effects: every *treatment contrast*  $\sum c_i \tau_i$  with  $\sum c_i = 0$  is of possible interest. All contrasts are *estimable* (can be linearly and unbiasedly

estimated) if and only if the block design is connected. For disconnected designs, all contrasts within the connected treatment subsets span the space of all estimable contrasts. For a given design d, we employ the *best* (minimum variance) linear unbiased estimators for contrasts. The variances of these estimators, and their covariances, though best for given d, are a function of d. In fact, if c is the vector of contrast coefficients  $c_i$  then the variance of contrast  $c'\tau = \sum c_i \tau_i$  is

$$\sigma^2 c' C_d^+ c$$

where  $C_d^+$  is the Moore-Penrose inverse of  $C_d$  (if  $C_d = \sum x_{di} E_{di}$  is the spectral decomposition of  $C_d$ , then  $C_d^+ = \sum_{x_{di} \neq 0} \frac{1}{x_{di}} E_{di}$ ). The information carried by  $C_d$  is the precision of our estimators: large information  $C_d$  corresponds to small variances as determined by  $C_d^+$ .

We wish to make variances small through choice of d. That is, we choose d so that  $C_d^+$  is (in some sense) small. Design optimality criteria are real-valued functions of  $C_d^+$  that it is desirable to minimize. Obviously a design criterion may also be thought of as a function of d itself, which we do when convenient.

With this background, let us turn now to what has been implemented for the external representation of statistical\_properties:

```
statistical_properties = element statistical_properties {
    attribute precision { xsd:positiveInteger } ,
    canonical_variances ? ,
    pairwise_variances ? ,
    optimality_criteria ? ,
    other_ordering_criteria ? ,
    canonical_efficiency_factors ? ,
    functions_of_efficiency_factors ? ,
    robustness_properties ?
}
```

The elements of statistical\_properties are quantities which can be calculated starting from the information matrix  $C_d$ .

## 7.6.1 Canonical variances

The  $v \times v$  symmetric, nonnegative definite matrix  $C_d$  is never of full rank; its maximal rank is v - 1, which is achieved exactly when the block design d is connected. Denote the v - 1 ordered, largest eigenvalues of  $C_d$  by

$$x_{d1} \le x_{d2} \le \dots \le x_{d,v-1}$$

Design d is connected if and only if  $x_{d1} > 0$ . The corresponding nonzero eigenvalues of  $C_d^+$  are the inverses of the nonzero  $x_{di}$ 's ; for a connected design these are

$$z_{d1} \ge z_{d2} \ge \dots \ge z_{d,v-1}$$

The  $z_{di}$  are called the *canonical variances*. They are the variances of a set of contrasts whose vectors of coefficients are any orthonormal set of eigenvectors of  $C_d$  orthogonal to the all-ones vector. We define a full set of v-1 canonical variances even for disconnected designs, in which case some of the  $z_{di}$  are taken as infinity. An infinite canonical variance corresponds to a contrast which is not estimable.

Many of the commonly used design optimality criteria are based on the canonical variances. Because of their importance they have merited an element, canonical\_variances, in the external representation. Infinite values are recorded there as "not\_applicable" and, as already explained, correspond to zero values of  $x_{di}$ 's.

#### 7.6.2 Pairwise variances

In statistical practice, some experiments focus on comparing the effect of each treatment to each other treatment; these are the *elementary contrasts*  $\tau_i - \tau_{i'}$ . The variances  $v_{dii'}$  of the elementary contrasts for a connected design d, aside from the constant  $\sigma^2$ , are

$$v_{dii'} = c_{dii}^+ + c_{di'i'}^+ - 2c_{dii'}^+$$

for  $1 \leq i < i' \leq v$ , where  $c_{dii'}^+$  is the general element of  $C_d^+$ . Several optimality criteria are based on the v(v-1)/2 numbers  $v_{dii'}$ , called *pairwise variances*. Moreover, partial balance properties are reflected in the  $v_{dii'}$ . For these reasons, **pairwise\_variances** is also an element in the external representation. For disconnected designs some elementary contrasts are not estimable; in the external representation, the corresponding values  $v_{dii'}$  are recorded as "not\_applicable."

### 7.6.3 Optimality criteria

We are now in a position to define the design optimality\_criteria that have been implemented.

### phi\_0

 $\Phi_0 = \sum \log(z_{di})$ 

This is the log of the product of the canonical variances, called the D-criterion (for "determinant"). The product is proportional to the volume of the confidence ellipsoid for joint estimation of the canonical contrasts.

#### phi\_1

 $\Phi_1 = \sum z_{di}/(v-1)$ 

This is the arithmetic mean of the canonical variances, called the Acriterion (for "average"). It is also proportional to the average of the v(v-1)/2 pairwise variances  $v_{dii'}$ .

## phi\_2

 $\Phi_2 = \sum z_{di}^2 / (v - 1)$ 

This is the mean of the squared canonical variances. For any fixed value of  $\Phi_1$  this is minimized when the  $z_{di}$  are as close as possible in the square error sense. Thus it is a measure of *balance* of the design. A design is said to be *variance balanced* when all normalized treatment contrasts are estimated with the same variance. This occurs if and only if all the  $z_{di}$  are equal, which gives the smallest conceivable (and often unattainable) value for  $\Phi_2$  for fixed  $\Phi_1$ . Among binary, equiblocksize designs, only balanced incomplete block designs achieve equality of the  $z_{di}$ .

## maximum\_pairwise\_variances

The largest pairwise variance  $(\max(v_{dii'}))$ , called the MV-criterion (for "maximum variance"). This is a minimax criterion: minimize the maximum loss (as measured by variance) for estimating the elementary contrasts.

### E\_criteria

 $z_{d1} + z_{d2} + \ldots + z_{di}$ 

The sum of the *i* largest canonical variances, called the  $E_i$  criterion.  $E_1$  is usually called "the" E-criterion; minimization of  $E_1$  is minimization of the worst variance over all possible normalized treatment contrasts.

 $E_1$  is the counterpart of maximum\_pairwise\_variances for the set of all contrasts. More generally, minimization of  $E_i$  is minimization of the sum of the i worst variances over all possible sets of i normalized treatment contrasts whose estimators are uncorrelated. Thus the  $E_i$ are a family of minimax criteria.  $E_{v-1}$  is equivalent to  $\Phi_1$ . A design which minimizes all of the  $E_i$  for i = 1, ..., v - 1 is Schur-optimal (it minimizes all Schur-convex functions of the canonical variances).

#### 7.6.4Other ordering criteria

In addition to the optimality criteria just listed, we also implement several ordering criteria for block designs (optimality criteria are ordering criteria that meet conditions described fully in a later subsection).

#### no\_distinct\_canonical\_variances

The number of distinct  $z_{di}$ . For balanced incomplete block designs this value is 1. A balance criterion; the fewer variances a design produces, the easier are the results to understand.

#### max\_min\_ratio\_canonical\_variances

The ratio of largest to smallest canonical variance  $(z_{d1}/z_{d,v-1})$ , called the canonical variance ratio. Again, the value for a balanced incomplete block design is 1. Values close to one correspond to variances that are quite similar.

#### no\_distinct\_pairwise\_variances

The number of distinct  $v_{dii'}$ . Analogous to no\_distinct\_canonical\_variances, but for pairwise variances rather than canonical variances.

#### element max\_min\_ratio\_pairwise\_variances

The ratio of largest to smallest pairwise variance  $(\max(v_{dii'}) / \min(v_{dii'}))$ , called the *pairwise variance ratio*. Analogous to max\_min\_ratio\_canonical\_variances, but for pairwise variances rather than canonical variances.

## trace\_of\_square

 $\sum z_{di}^{-2} = \sum x_{di}^2$ . The trace of the square of  $C_d$ . This is called the S-criterion. Typically invoked as part of an (M,S)-optimality argument (minimize S subject to maximizing the trace of  $C_d$ ). No direct statistical interpretation, though usually leads to reasonably "good" designs.

It was mentioned above that a complete block design (each block size is v and each treatment is assigned to one unit in each block) is a "good" design. Now we state why. Over all possible assignments of v treatments to b blocks of size v, a complete block design minimizes *all* of the criteria defined above (save for  $tr(C_d^2)$ , which it minimizes subject to the mean of the unsquared components). The same statement holds for a balanced incomplete block design for constant block size less than v (whenever a BIBD exists). Otherwise, the optimal block design problem can be quite tricky, with such uniform optimality hard to come by.

An optimality\_value for any of the optimality criteria above has three elements: its numerical value and two associated numbers absolute\_efficiency and calculated\_efficiency (for other\_ordering\_criteria, the same concepts are implemented under the names absolute\_comparison and calculated\_comparison so are not separately discussed here - see the later subsection on design orderings). Given any two designs,  $d_1$  and  $d_2$  say, they can be compared on any of the listed optimality criteria. The *relative efficiency* of design  $d_2$  with respect to criterion  $\Phi$ , compared to design  $d_1$ , is  $\Phi(d_1)/\Phi(d_2)$ . If  $d_1$  is in fact an *optimal* design as measured by  $\Phi(d_1 \text{ minimizes } \Phi(d) \text{ over all } d)$ , then the relative efficiency of any d compared to  $d_1$  is the absolute\_efficiency of d. Both of these efficiencies are between 0 and 1, with smaller criterion values corresponding to larger efficiencies; the absolute efficiency of an optimal design is 1.

The concept of absolute efficiency depends on what is meant by the phrase "all d". It has already been explained that comparisons are for designs with the same v, b, and block sizes. In the external representation, an absolute\_efficiency is for the class of all binary designs with the same v, b, and block size distribution, called the *reference universe*. When the minimum criterion value over the reference universe is not known. absolute\_efficiency takes the value "unknown." For a disconnected design absolute\_efficiency takes the value "0" regardless of whether the optimal value is known or not. It happens, only rarely, that a smaller value of a criterion can be found for a nonbinary design with the same v, b, and block sizes, in which case the absolute\_efficiency of the nonbinary design will be greater than 1. Nonbinary designs are not at present considered in the external representation. Relative efficiencies when the best value over the reference universe is not known, or within a subclass of the reference universe, can be calculated on a case-by-case basis; in external representation terminology, this is a calculated\_efficiency. For instance, one may wish to compare only resolvable designs. calculated\_efficiency takes the value "0" for all disconnected designs.

## 7.6.5 Efficiency factors

There is another set of values, the canonical\_efficiency\_factors, that are used to evaluate a design but which has not yet been discussed. Let  $r_i$ be the number of units receiving treatment *i* (this is the general diagonal element of  $A'_dA_d$ ) and let *R* be the diagonal matrix with the  $\sqrt{r_i}$  along the diagonal. The canonical efficiency factors

$$e_{d1} \le e_{d2} \le \dots \le e_{d,v-1}$$

for design d are the v - 1 largest eigenvalues of  $F_d = R^{-1}C_dR^{-1}$ . The remaining eigenvalue of  $F_d$  is 0.

In the incomplete block design, the variance of the estimator of  $x'\tau$  is equal to  $x'C_d^-x\sigma_{\text{IBD}}^2$ , while the variance in a completely randomized design with the same replication is  $x'R^{-2}x\sigma_{\text{CRD}}^2$ , where the two values of  $\sigma^2$  are the variances per plot in the incomplete block design and the completely randomized design respectively. Therefore the relative efficiency is

$$\frac{x'R^{-2}x}{x'C_d^-x} \times \frac{\sigma_{\rm CRD}^2}{\sigma_{\rm IBD}^2}$$

The first part of this, which depends on the design but not on the values of the plot variances, is called the *efficiency factor* for the contrast  $x'\tau$ . Put  $R^{-1}x = u$ . Then the efficiency factor for  $x'\tau$  is

$$\frac{u'u}{u'F_d^-u},$$

which is equal to  $\varepsilon$  if u is an eigenvector of F with eigenvalue  $\varepsilon$ .

Since  $F_d$  is symmetric, it can orthogonally diagonalized. The contrast  $x'\tau$  is called a *basic contrast* if x = Ru for an eigenvector u of  $F_d$  which is not a multiple of  $Ru_0$ , where  $u_0$  is the all-1 vector. The basic contrasts span the space of all treatment contrasts; moreover, if  $u_1$  is orthogonal to  $u_2$  then the estimators of  $(Ru_1)'\tau$  and  $(Ru_2)'\tau$  are uncorrelated (and independent if the errors are normally distributed).

Each efficiency factor lies between 0 and 1; at the extremes are contrasts that cannot be estimated (efficiency factor = 0) and contrasts that are estimated just as well as in an unblocked design with the same  $\sigma^2$  (efficiency factor

= 1). Thus  $1 - e_{di}$  is the proportion of information lost to blocking when estimating a corresponding basic contrast (or any contrast in its eigenspace);  $e_{di}$  is the proportion of information retained. Design *d* is disconnected if and only if  $e_{d1} = 0$ .

The comparison to a completely randomized design with the same replication numbers is the key concept here. Efficiency factors evaluate design dover the universe of all designs with the same replications  $r_1, \ldots, r_v$  as d, constraining the earlier discussed reference universe of competitors with the given v and block size distribution. This constrained universe of comparison is typically justified as follows: the replication numbers have been purposefully chosen (and thus fixed) to reflect relative interest in the treatments, or the replication numbers are forced by the availability of the material (for example, scarce amounts of seed of new varieties but plenty of the control varieties), so the task is to determine a best (in whatever sense) design within those constraints. The idealized best (in every sense) is the completely randomized design (no blocking) so long as this does not increase the variance per plot. Though experimental material at hand has forced blocking, the unobtainable CRD can still be used as a fixed basis for comparison.

Variances of contrasts estimated with a CRD exactly mirror the selected sample sizes. If the replication numbers are intended to reflect relative interest in treatments, then a reasonable design goal is to find d for which variances of all contrast estimators enjoy the same relative magnitudes as in the CRD. This is exactly the property of *efficiency balance*: design d is *efficiency balanced* if its canonical efficiency factors are all equal:  $e_{d1} = e_{d2} = \ldots = e_{d,v-1}$ .

For equal block sizes k (< v), the only equireplicate, binary, efficiency balanced designs are the BIBDs. Unfortunately, an unequally replicated design cannot be efficiency balanced if the block sizes are constant and it is binary. Thus in many instances the best hope is to approximate the relative interest intended by the choice of sample sizes. Approximating efficiency balance (seeking small dispersion in the efficiency factors) will then be a design goal, typically in conjunction with seeking a high overall efficiency factor as measured through one or more summary functions of the canonical efficiency factors. The harmonic mean of the canonical efficiency factors (see below) is often called "the" efficiency factor of a design; if the value is 0.87, for instance, then use of blocks has resulted in an overall 13% loss of information.

For an equireplicate design (all  $r_i$  are equal—to r say) the canonical effi-

ciency factors are just 1/r times the inverses of the canonical variances; some statisticians consider them a more interpretable alternative to the canonical variances in this case. If all the efficiency factors are 1, the design is *fully efficient*, a property achieved in the equiblocksize case (with  $k \leq v$ ) only by complete block designs. Consequently, efficiency factors for equireplicate designs can also be interpreted as summarizing the loss of information when using incomplete blocks (block sizes smaller than v) rather than complete blocks.

The external representation contains the following commonly used summaries\_of\_efficiency\_factors. In terms of these measures, an optimal design is one which *maximizes* the value. Each summary measure induces a design ordering which is identical to that for one of the optimality\_criteria above, based on the canonical variances, *provided* the set of competing designs is restricted to be equireplicate. More generally, these measures should only be used to compare designs with the same replication numbers.

## harmonic\_mean

 $(v-1)/\sum (1/e_{di})$ 

This is the harmonic mean of the efficiency factors. Equivalent to (produces the same design ordering as)  $\Phi_1$  in the equireplicate case.

# geometric\_mean

 $exp(\sum log(e_{di})/(v-1))$ 

This is the geometric mean of the efficiency factors. Equivalent to (produces the same design ordering as)  $\Phi_0$  in the equireplicate case.

## minimum

The smallest efficiency factor  $(e_{d1})$ . Equivalent to  $E_1$  in the equireplicate case.

The Introduction gives an example of a block design which is called the Fano plane. It is a BIBD for 7 treatments in 7 blocks of size 3. As with any BIBD, it is pairwise\_balanced, variance\_balanced, and efficiency\_balanced, and it is optimal with respect to all of the optimality\_criteria over its entire reference universe. Here are all of the statistical\_properties, that have been discussed so far, for this example:

```
</canonical_variances>
<pairwise_variances>
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    ordered="true">
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                </entire_domain>
            </preimage>
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   </phi_0>
    <phi_1>
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        <calculated_efficiency><z>1</z></calculated_efficiency>
   </phi_1>
   <phi_2>
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   </phi_2>
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        </E_value>
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        </E_value>
```

```
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            <calculated_efficiency><z>1</z></calculated_efficiency>
        </E_value>
        <E_value index="4">
           <value><d>1.71428571</d></value>
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            <calculated_efficiency><z>1</z></calculated_efficiency>
        </E value>
        <E_value index="5">
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            <absolute_efficiency><z>1</z></absolute_efficiency>
            <calculated_efficiency><z>1</z></calculated_efficiency>
        </E_value>
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            <value><d>2.57142857</d></value>
            <absolute_efficiency><z>1</z></absolute_efficiency>
            <calculated_efficiency><z>1</z></calculated_efficiency>
        </E_value>
    </E_criteria>
</optimality_criteria>
<other_ordering_criteria>
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        <calculated_comparison><z>1</z></calculated_comparison>
    </trace_of_square_of_C>
    <max_min_ratio_canonical_variances>
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```

```
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    </other_ordering_criteria>
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        </harmonic_mean>
        <geometric_mean alias="D">
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        </geometric_mean>
        <minimum alias="E">
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        </minimum>
    </functions_of_efficiency_factors>
</statistical_properties>
```

# 7.6.6 Robustness properties

Experiments do not always run successfully on all experimental units. In the fertilizer/tobacco example above, if midway through the growth period one of the pots is accidentally broken, then one experimental unit has been "lost." One is effectively left with a *different* block design, with different properties than the one initiated.

The concept of *robustness* of a block design is here considered as its ability to maintain desirable statistical properties under loss of individual plots or entire blocks. Such a loss is catastrophic if the design becomes disconnected. Less than catastrophic but of genuine concern are losses in the information provided by the design, as measured by various optimality criteria. The two elements of **robustness\_properties** accommodate these two perspectives.

The element robust\_connected makes the statement *The design is connected under all possible ways in which* number\_lost *of* category\_lost *can be removed.* If the reported value of number\_lost is known to be the largest integer for which this statement is true then is\_max takes the value "true" and otherwise takes the value "unknown" (the value "false" is not allowed).

The element robust\_efficiencies reports A, E, D, and MV efficiencies for a given number (number\_lost) of plots or blocks (category\_lost) removed

from the design. The efficiencies can be calculated from two different perspectives. If loss\_measure = "average" then the criterion value used is the average of all its values over all possible deletions of the type and number prescribed. If loss\_measure = "worst" then the criterion value used is the maximum of all its values over all possible deletions of the type and number prescribed.

Balance measures have not been incorporated under robust\_efficiencies. This is because designed balance is typically severely affected by plot/block loss and in ways that need have no relation to treatment structure.

The calculations associated with the values reported here can be quite expensive.

## 7.6.7 Computational details

As has already been explained, the elements of statistical\_properties are quantities which can be calculated starting from the information matrix  $C_d$ . There are three fundamental calculations: the canonical variances, the pairwise variances, and the canonical efficiency factors.

The canonical variances are the inverses of the eigenvalues of  $C_d$ , eigenvalues of zero corresponding to canonical variances of  $\infty$ . Thus we need the roots of the polynomial  $|C_d - xI| = 0$ . As  $C_d$  is a rational matrix, this polynomial admits a factorization into irreducible factors over the rational field. Thus, in theory, the multiplicities of the canonical variances can be determined exactly, even if some of the values themselves are irrational. If the eigenvalues of  $C_d$  are numerically extracted directly without factoring the characteristic polynomial, then the problem of inexact counts of those eigenvalues can arise.

Pairwise variances are defined above in terms of the Moore-Penrose inverse  $C_d^+$  of  $C_d$ :  $v_{dii'} = c_{dii}^+ + c_{di'i'}^+ - 2c_{dii'}^+$ . In fact, any generalized inverse  $C_d^-$  of  $C_d$  can be used, from which  $v_{dii'} = c_{dii}^- + c_{di'i'}^- - 2c_{dii'}^-$ . Let J be an all-ones matrix. If d is connected, then  $C_d + aJ$  is invertible for any  $a \neq 0$  and  $C_d^- = (C_d + aJ)^{-1}$  is a generalized inverse of  $C_d$  (the same operation can be carried out for the connected components of  $C_d$  if d is disconnected). Thus pairwise variances can be calculated by inversion of a rational, nonsingular matrix.

Efficiency factors are defined as eigenvalues of the matrix  $F_d = R^{-1}C_dR^{-1}$ , which can certainly be irrational. Extracting the roots of  $N_dK^{-1}N'_d$  with respect to  $R^2$ , that is, solving the equation  $|N_d K^{-1} N'_d - \mu R^2| = 0$ , produces values  $\mu_{di}$  for i = 1, ..., v satisfying  $\mu_{dv} = 0$  and otherwise  $\mu_{di} = 1 - e_{di}$ . Thus efficiency factors can be found by extracting roots of a symmetric, rational matrix, involving the same computational issues as for the canonical variances.

The number of infinite canonical variances equals the number of connected components of d less 1 (this being zero for any connected designs). Numerical extraction of eigenvalues of  $C_d$  can potentially produce, at a given level of precision, values indistinguishable from zero that are in actuality positive, consequently producing an erroneous number of infinite canonical variances. This approximation error is prohibited by cross-checking against the **connected** indicator.

# 7.6.8 Design orderings based on the information matrix

The external representation implements optimality criteria and other ordering criteria as aids in judging statistical properties of of members of a class of block designs. Definitions and motivating principles for these two classes of criteria are given here.

Denote by C the class of information matrices for the class of designs D under consideration, that is,

$$\mathcal{C} = \{C_d : d \in \mathcal{D}\}.$$

If g map elements of C to a subset of the reals plus  $\infty$ , then g provides an ordering on d:

$$d_1 \ge_g d_2 \iff g(C_{d1}) \le g(C_{d2})$$

Usually  $\mathcal{D}$  is our reference universe, but need not be so. In any case  $\mathcal{D}$  is finite and  $g(C_d) = \infty$  if and only if d is disconnected.

While it is trivial to define ordering functions g, what does it mean for a function  $g: \mathcal{C} \to \mathcal{R}$  to be an *optimality criterion*? Any ordering of information matrices could be allowed, but not all orderings reflect a reasonable statistical concept of optimality. We work here towards appropriate definitions.

The first fundamental consideration is that of relative interest in the v members of the treatment set. Let  $\mathcal{P}$  be the class of  $v \times v$  permutation matrices.

If treatments are of equal interest, then order g should satisfy the symmetry condition

$$g(C_d) = g(PC_dP')$$
 for every  $P \in \mathcal{P}$ .

Only g satisfying this condition are considered here.

Another fundamental principle arises from the nonnegative definite ordering on information matrices:

$$C_{d_1} \geq_{nnd} C_{d_2} \iff C_{d_1} - C_{d_2}$$
 is nonegative definite

Now  $C_{d_1} \geq_{nnd} C_{d_2} \iff C_{d_2}^+ \geq_{nnd} C_{d_1}^+$  so this ordering says  $\operatorname{var}_{d_1}(\widehat{l'\tau}) \leq \operatorname{var}_{d_2}(\widehat{l'\tau})$  for every contrast  $l'\tau$ . A reasonable restriction to place on an optimality criterion g is that it respect the nonnegative definite ordering:

$$C_{d_2}^+ \ge_{nnd} C_{d_1}^+ \Rightarrow g(C_{d_1}) \le g(C_{d_2})$$

*Fact*: In the reference universe of all binary block designs with v treatments and fixed block size distribution,  $C_{d_2}^+ \geq_{nnd} C_{d_1}^+ \iff C_{d_1} = C_{d_2}$ 

*Proof*: The trace  $tr(C_d)$  is fixed for all d in the reference universe. Consequently  $C_{d_1} \geq_{nnd} C_{d_2}$  says that  $C_{d_1} - C_{d_2}$  is a nonnegative definite matrix with zero trace, that is, it is the zero matrix.

Thus the nonnegative definite ordering does not distinguish among ordering functions g for the reference universe. While the external representation does not currently include nonbinary designs, we take as part of our definition that an optimality criterion g must respect the nonnegative definite ordering; effectively, it must be able to make this fundamental distinction in the larger class of *all* designs with the same v and block size distribution. A criterion that cannot do this has little (if any) capacity to detect inflated variances.

Typically one wishes to consider not arbitrary functions on the matrices  $C_d$ , but functions of some characteristic(s) of those matrices. Of particular interest are the lists of canonical variances and pairwise variances. A criterion which is a function of a list of values should respect orderings of lists, as follows. A list  $L_d$  of s real values calculated from  $C_d$  may be thought of as the uniform probability distribution  $p(l) = \frac{1}{s}$  for each  $l \in L_d$ . Probability distributions may be stochastically ordered: the distribution of X is stochastically larger than that of Y, written  $X \ge_s Y$ , if  $\Pr(X \le a) \le \Pr(Y \le a)$ for every a. Thus define  $L_{d_2}$  to be stochastically larger than  $L_{d_1}$ , written  $L_{d_2} \ge_s L_{d_1}$ , if  $|L_{d_2} \le a| \le |L_{d_1} \le a|$  for every a. Criterion g respects the stochastic ordering with respect to list L if

$$L_{d_2} \ge_s L_{d_1} \Rightarrow g(C_{d_1}) \le g(C_{d_2})$$

The nnd order on information matrices (or their M-P inverses) implies the stochastic order on both the lists of canonical variances and the lists of pairwise variances.

Fact: In the reference universe of all binary block designs with v treatments and fixed block size distribution, if L is the list of canonical variances, then  $L_{d_2} \geq_s L_{d_1} \iff L_{d_2} = L_{d_1}$ .

*Proof*: This follows from fixed trace of the information matrix in the reference universe, and that element-wise inversion of nonnegative lists reverses the stochastic ordering.

Thus every ordering criterion that is a function of the list of canonical variances trivially respects the stochastic order over the binary class. This may not be so for a criterion based on the list of pairwise variances.

A weaker ordering of lists than stochastic ordering, which is of some interest and which is not trivially respected in the binary class, is the *weak majorization ordering*. Let  $L_{d[i]}$  be the  $i^{th}$  largest member of list  $L_d$ . Define  $L_{d_2}$  to weakly majorize  $L_{d_1}$ , written  $L_{d_2} \ge_m L_{d_1}$ , if  $\sum_{i=1}^t L_{d_2[i]} \ge \sum_{i=1}^t L_{d_1[i]}$  for every  $t = 1, 2, \ldots, s$ . If also equality of the two sums holds at t = s, then  $L_{d_2}$ is said simply to *majorize*  $L_{d_1}$ . Criterion g respects the weak majorization ordering with respect to list L if

$$L_{d_2} \ge_m L_{d_1} \Rightarrow g(C_{d_1}) \le g(C_{d_2}).$$

The weak majorization ordering is respected by every function of the form  $g(C_d) = \sum_{i=1}^{s} h(L_{di})$  for continuous, increasing, convex h.

For any connected design d, the inverses of the canonical variances are the eigenvalues of the information matrix  $C_d$ . Now the list of eigenvalues has constant sum for all d in the reference universe; for these lists, majorization and weak majorization are equivalent. Moreover, if two lists of eigenvalues are ordered by majorization, then the corresponding lists of canonical variances are ordered by weak majorization. Consequently, weak majorization can sometimes be determined for canonical variances over the reference universe via the corresponding eigenvalues of information matrices.

Relationships among the three ordering principles discussed are

nnd ordering  $\Rightarrow$  stochastic ordering  $\Rightarrow$  weak majorization ordering

the latter two for either the pairwise variances or the canonical variances. None of the implications can in general be reversed.

We call a symmetric ordering criterion an *optimality criterion* if (1) it preserves the nnd definite ordering of information matrices over the generalized universe of all designs for given v and block size distribution, and (2) it admits direct interpretation as a summary measure of magnitude of variances of one or more treatment contrast estimators. Each of the functions in **optimality\_criteria** possesses these two properties.

Ordering criteria can fall outside this scope yet still be of interest, such as those provided in the element other\_ordering\_criteria. These functions, discussed next, typically fail on both requirements for an optimality criterion, but may preserve orderings in restricted classes.

The S-criterion  $(\operatorname{tr}(C_d^2))$  is typically employed as the second step in a socalled (M, S)-optimality argument: first maximize  $\operatorname{tr}(C_d)$  (that is, restrict to the binary class - our reference universe), then minimize S. Within the binary class, S preserves the weak majorization order on the canonical variances; outside of that class, it is possible to find considerably smaller values of S, though inevitably at considerable cost on one or more optimality criteria. Thus S may be viewed as an ordering criterion suitable for use in restricted classes, and/or in a subsidiary role to one or more optimality criteria in a multi-criterion design screening.

The function max\_min\_ratio\_canonical\_variances preserves the weak majorization order over the binary class (indeed within any fixed  $tr(C_d)$  class), and max\_min\_ratio\_pairwise\_variances preserves the majorization order over that class. Both suffer the same defects as S outside the reference universe. Each of these three criteria is a summary measure of scatter of variances, not of magnitude; minimizing over too large a class will reduce scatter at the cost of increasing magnitude.

Two additional ordering criteria implemented are the support sizes of the distributions of canonical variances and pairwise variances. These, too, can be informative as subsidiary criteria in a multi-criterion design search, but because they do not employ the values in the corresponding distributions, no\_distinct\_canonical\_variances and no\_distinct\_pairwise\_variances cannot be guaranteed to preserve (outside of the reference universe) any of the list orderings discussed. Like S and the variance ratios, these measures give information on scatter in a list of variances, and thus are fairly called *balance criteria*.

Included with other\_ordering\_criteria are absolute\_comparisons and calculated\_comparisons. These serve the same role, and are computed with the same rules, as absolute\_efficiencies and calculated\_efficiencies for optimality\_criteria. Because other\_ordering\_criteria typically do not measure magnitude of variance, we do not consider it correct terminological usage to call their relative values "efficiencies."

# 8 Lists of Block Designs

A list of block designs is essentially what the name implies. However, the listed designs must be distinct, and we allow assertions to be made about this list; in particular, it will be possible to say

- the designs in the list are pairwise non-isomorphic;
- these are all the designs with such-and-such properties.

Here is the schema definition for the *list\_of\_designs* element which is the root element of any valid external representation document.

```
list_of_designs = element list_of_designs {
    attribute dtrs_protocol { "1.1" },
    attribute design_type { "block_design" | "latin_square" },
    attribute pairwise_nonisomorphic { "true" | "false" | "unknown" },
    attribute no_designs { xsd:nonNegativeInteger | "unknown" } ?,
    attribute precision { xsd:positiveInteger } ?,
    list_definition ?,
    ( block_design | latin_square ) *,
    info ?
}
```

There are three compulsory attributes:

```
dtrs_protocol
```

It will be used by applications to check compliance of documents and of themselves. It must contain a fixed string representing the current protocol version of external representation schema.

In the future, the minor version number will be incremented when backward compatible minor changes have been made. That means that older documents satisfying previous protocols with the same major version number remain valid under the new protocol. The corresponding requirement for implementations is that an implementation in compliance with a given protocol version should be able to deal with any document of the same major and a lower protocol version.

The major version will be incremented between not entirely compatible versions or when significant new structures have been introduced.

## design\_type

Currently the only implemented design type is (binary) block design which is indicated by the string "block\_design".

## pairwise\_nonisomorphic

This is "true" if the designs in the list are known to be pairwise nonisomorphic, "false" if they are known not to be, and "unknown" otherwise.

The optional list\_definition component will be used to define *list in*variants and to formulate queries to the database. These concepts are the subjects of future development.

# 9 Implementation Policies

## (Under development)

The external representation for block designs gives the implementor a great deal of choice about what to include when specifying a block design and its properties. Here we record our policies about what (and what not) to include in certain cases:

## How far to go with point\_concurrences?

If the given block design is not a *t*-design (with  $t \ge 2$ ), then include the *k*-wise point concurrences only for k = 1 and (unless there is just one point) k = 2. In both cases, the full preimage should be given (which may be entire\_domain). This policy gives the replication number for each point and the pairwise point concurrences. If the given block design D is a *t*-design (with t = 2) then include the *k*wise point concurrences for k = 1, 2, ..., max(t) for which D is a *t*design. Again, full preimages should be given and they are all, of course, entire\_domain.

## How far to go with block\_concurrences?

Include the k-wise block concurrences for k = 1 and (unless there is just one block) k = 2. In both cases, preimages should be collapsed to preimage cardinalities. This policy gives the sizes of the blocks, the number of blocks of each size, the sizes of the pairwise intersections of blocks, and the number of pairs of blocks giving each intersection size.

# How far to go with t\_wise\_balanced?

This is analogous to point\_concurrences. If the given block design D is not a t-design (with t = 2), then normally include whether or not D is t-wise balanced only for t = 1 and t = 2. Otherwise, include this information for t = 1, 2, ..., max(t) for which D is a t-design. Note that this maximum t is recorded in the t\_design indicator.

# References

- R. A. Bailey, P. J. Cameron, P. Dobcsányi, J. P. Morgan, L. H. Soicher: Designs on the Web, preprint available at: http://designtheory.org/library/preprints/
- [2] T. Beth, D. Jungnickel, H. Lenz: *Design Theory*, Volumes 1 and 2 (Second edition), Cambridge University Press, 1999.
- [3] T. Calinski, S. Kageyama: Block Designs: A Randomization Approach, Lecture Notes in Statistics 150, Springer, New York, 2000.
- [4] C.J. Colbourn, J.H. Dinitz (Editors): The CRC Handbook of Combinatorial Designs, CRC Press, 1996.
- [5] K. R. Shah, B. K. Sinha: *Theory of Optimal Designs*, Springer, New York, 1989.
- [6] Relax NG Schema Language for XML, http://relaxng.org/

# A design.rnc

```
# $Id: design.rnc,v 1.133 2003/12/12 14:16:43 peter Exp $
# External Representation of Designs
#
# Version: 1.1
#
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# Leonard Soicher
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# Please send comments, questions, bug reports to:
#
#
       extrep@designtheory.org
#
default namespace dtrs = "http://designtheory.org/xml-namespace"
datatypes xsd = "http://www.w3.org/2001/XMLSchema-datatypes"
### list of designs ###
start = list_of_designs # root of every ext-rep document
list_of_designs = element list_of_designs {
```

```
{ "1.1" } ,
    attribute dtrs_protocol
                                    { "block_design" | "latin_square" } ,
    attribute design_type
    attribute pairwise_nonisomorphic { "true" | "false" | "unknown" } ,
                                   { xsd:nonNegativeInteger | "unknown" } ? ,
    attribute no_designs
    attribute precision
                                    { xsd:positiveInteger } ? ,
    list_definition ? ,
    # no designs should be repeated.
    ( block_design | latin_square ) * ,
    info ?
}
# query language components
# (place holder only, to be defined later)
list_definition = element list_definition {
   list_invariants ,
   no_pairwise_nonisomorphic
}
list_invariants = element list_invariants { empty }
no_pairwise_nonisomorphic = element no_pairwise_nonisomorphic { empty }
### common components for all type of designs
# elementary objects
unknown = element unknown { empty }
not_applicable = element not_applicable { empty }
z = element z { xsd:integer }
q = element q { text } # must be in the format a/b
d = element d { xsd:decimal }
# functions on indices
function_on_indices = element function_on_indices {
                               { "points" | "blocks" } ,
   attribute domain
    attribute n
                               { xsd:nonNegativeInteger } ,
                               { "true" | "unknown" } ,
    attribute ordered
   attribute image_cardinality { xsd:positiveInteger } ? ,
   attribute precision { xsd:positiveInteger } ? ,
    attribute title
                               { text } ? ,
    ( map + | blank )
}
function_on_ksubsets_of_indices = element function_on_ksubsets_of_indices {
    attribute domain_base
                               { "points" | "blocks" } ,
```

```
{ xsd:nonNegativeInteger } ,
    attribute n
                                { xsd:nonNegativeInteger } ,
    attribute k
                                { "true" | "unknown" } ,
    attribute ordered
    attribute image_cardinality { xsd:positiveInteger } ?
    attribute precision
                                { xsd:positiveInteger } ? ,
    attribute title
                                { text } ? ,
    ( map + | blank )
}
# if <blank> is given instead of <map>-s, 'image_cardinality' must be specified
map = element map {
    ( preimage | preimage_cardinality | blank )
    element image { z \mid d \mid q \mid not_applicable }
}
preimage = element preimage {
   z +
    element ksubset { z+ } +
    entire_domain
}
preimage_cardinality = element preimage_cardinality { z }
blank = element blank { empty }
entire_domain = element entire_domain { empty }
# permutation groups and their properties
permutation_group = element permutation_group {
    attribute degree { xsd:positiveInteger } ,
    attribute order { xsd:positiveInteger } ,
    attribute domain { "points" },
    generators ,
    permutation_group_properties?
}
permutation_group_properties = element permutation_group_properties {
    element primitive {
attribute flag { "true" | "false" }
    } ?
```

```
element generously_transitive {
attribute flag { "true" | "false" }
   } ?
    element multiplicity_free {
attribute flag { "true" | "false" }
    } ?
    element stratifiable {
attribute flag { "true" | "false" }
    } ?
    element no_orbits {
attribute value { xsd:positiveInteger }
    } ?
    element degree_transitivity {
attribute value { xsd:nonNegativeInteger }
    } ?
    element rank {
attribute value { xsd:positiveInteger }
    } ?
    cycle_type_representatives ?
}
cycle_type_representatives = element cycle_type_representatives {
    cycle_type_representative +
}
cycle_type_representative = element cycle_type_representative {
    permutation ,
    element cycle_type {
attribute ordered { "true" } ,
z+
    },
    element no_having_cycle_type { z } ?
}
generators = element generators {
    permutation *
}
```

```
permutation = element permutation { z+ }
# matrix
matrix = element matrix {
    attribute no_rows { xsd:positiveInteger } ,
    attribute no_columns { xsd:positiveInteger } ,
   attribute title
                    { text } ? ,
    row +
}
row = element row { (z | q | d)+ }
# <info> commonly used for all type of designs
info = element info {
    element creator {
element person { text } *
element software { text } *
    } + ,
    element reference { text } * ,
    element note { text } *
}
### block design ###
block_design = element block_design {
    attribute id { xsd:ID } ,
    attribute v { xsd:positiveInteger } ,
    attribute b { xsd:positiveInteger } ? ,
    attribute precision { xsd:positiveInteger } ? ,
    blocks ,
    point_labels ? ,
    indicators ? ,
    combinatorial_properties ? ,
    block_design_automorphism_group ? ,
    resolutions ? ,
    statistical_properties ? ,
    alternative_representations ? ,
    info ?
}
blocks = element blocks {
    attribute ordered { "true" } ,
```

```
block+
}
block = element block { z+ }
point_labels = element point_labels {
    z+
    element label { text } +
}
indicators = element indicators {
    element repeated_blocks {
attribute flag { "true" | "false" }
    } ?
    &
    element resolvable {
attribute flag { "true" | "false" }
   } ?
    &
    element affine_resolvable {
attribute flag { "true" | "false" },
attribute mu { xsd:positiveInteger } ?
    } ?
    &
    element equireplicate {
attribute flag { "true" | "false" } ,
attribute r { xsd:positiveInteger } ?
    } ?
    &
    element constant_blocksize {
attribute flag { "true" | "false" } ,
attribute k
            { xsd:positiveInteger } ?
    } ?
    &
    element t_design {
attribute flag { "true" | "false" } ,
attribute maximum_t { xsd:positiveInteger } ?
    } ?
    &
    element connected {
attribute flag { "true" | "false" } ,
attribute no_components { xsd:positiveInteger } ?
    } ?
    &
```

```
element pairwise_balanced {
attribute flag { "true" | "false" } ,
attribute lambda { xsd:positiveInteger } ?
   } ?
   &
   element variance_balanced {
attribute flag { "true" | "false" }
   } ?
   &
   element efficiency_balanced {
attribute flag { "true" | "false" }
   } ?
   &
   element cyclic {
attribute flag { "true" | "false" }
   } ?
   &
   element one_rotational {
attribute flag { "true" | "false" }
   } ?
}
combinatorial_properties = element combinatorial_properties {
   point_concurrences ? ,
   block_concurrences ? ,
   t_design_properties ? ,
   alpha_resolvable ? ,
   t_wise_balanced ?
}
block_concurrences = element block_concurrences {
    function_on_ksubsets_of_indices + # with domain_base="blocks"
}
point_concurrences = element point_concurrences {
   function_on_ksubsets_of_indices + # with domain_base="points"
}
t_design_properties = element t_design_properties {
    element parameters {
attribute t { xsd:positiveInteger } ,
attribute v { xsd:positiveInteger } ,
attribute b { xsd:positiveInteger } ,
attribute r { xsd:positiveInteger } ,
attribute k { xsd:positiveInteger } ,
```

```
attribute lambda { xsd:positiveInteger }
    } ?
    &
    element square {
attribute flag { "true" | "false" }
    } ?
    &
    element projective_plane {
attribute flag { "true" | "false" }
    } ?
    &
    element affine_plane {
attribute flag { "true" | "false" }
    } ?
    &
    element steiner_system {
attribute flag { "true" | "false" } ,
attribute t
            { xsd:positiveInteger } ?
    } ?
    &
   element steiner_triple_system {
attribute flag { "true" | "false" }
   } ?
}
index_flag = element index_flag {
    attribute index { xsd:nonNegativeInteger },
    attribute flag { "true" | "false" | "unknown" }
}
alpha_resolvable = element alpha_resolvable {
    index_flag +
}
t_wise_balanced = element t_wise_balanced {
    index_flag +
}
block_design_automorphism_group = element automorphism_group {
    permutation_group,# 'domain' must be "points"
    block_design_automorphism_group_properties ?
}
```

```
block_design_automorphism_group_properties = element automorphism_group_properties {
    element block_primitive {
```

```
attribute flag { "true" | "false" | "not_applicable" }
} ?
element no_block_orbits {
   attribute value { xsd:positiveInteger | "not_applicable" }
} ?
element degree_block_transitivity {
   attribute value { xsd:nonNegativeInteger | "not_applicable" }
} ?
}
resolutions = element resolutions {
    attribute pairwise_nonisomorphic { "true" | "false" | "unknown" } ,
   attribute all_classes_represented { "true" | "false" | "unknown" } ,
   resolution +
}
resolution = element resolution {
    function_on_indices,# with domain="blocks"
   resolution_automorphism_group ?
}
resolution_automorphism_group = element automorphism_group {
   permutation_group,# 'domain' must be "points"
   resolution_automorphism_group_properties?
}
resolution_automorphism_group_properties =
    element automorphism_group_properties { empty } # to be defined later
statistical_properties = element statistical_properties {
    attribute precision { xsd:positiveInteger } ,
    canonical_variances ? ,
   pairwise_variances ? ,
    optimality_criteria ? ,
    other_ordering_criteria ? ,
    canonical_efficiency_factors ? ,
   functions_of_efficiency_factors ? ,
   robustness_properties ?
    # all optional elements omitted if number of treatments=1
}
canonical_variances = element canonical_variances {
    attribute no_distinct { xsd:positiveInteger | "unknown" | "not_applicable" } ,
```

```
# no_distinct = "not_applicable" for disconnected designs
    attribute ordered { "true" | "unknown" } ,
    element value {
        attribute multiplicity { xsd:positiveInteger | "not_applicable" } ,
        ( d | q | z | blank | not_applicable )
    } +
    \ensuremath{\texttt{\#}} for a design with u connected components, there must be u-1 values
    # of "not_applicable"
    # if present as a value, "not_applicable" is largest if values ordered
}
pairwise_variances = element pairwise_variances {
    function_on_ksubsets_of_indices # with domain_base="points" and k="2"
7
optimality_criteria = element optimality_criteria {
    # These are functions either of
    # (i) the canonical variances z_1 > z_2 > \ldots > z_{v-1}, which are the
      inverses of the v-1 largest eigenvalues of the information matrix C
    #
    #
       (the inverse of zero being defined as infinity) or
    # (ii) the v(v-1)/2 pairwise variances v_{ij}=d_{ii}+d_{jj}-2d_{ij}
       for 1<=i<j<=v where d_{ij} is the general element of C<sup>+</sup> (the
    #
       Moore-Penrose inverse of C)
    #
   # In the connected case, the canonical variances are exactly the
   # nonzero eigenvalues of C^+; in the general case, they are the
   # nonzero eigenvalues of C^+ in addition to u-1 values of infinity,
   # where u is the number of connected components
   # Smaller values correspond to "better" designs
    # Efficiencies (see absolute_efficiency) are stored when an optimal
    # design is known WITHIN THE BINARY CLASS, in which case the value
    # is relative to the best binary design. It is thus possible that
    # a nonbinary design could be "superefficient", ie have efficiency
    # larger than 1.
    #
   # value = actual numerical value of the function for this design
    # absolute_efficiency = (value for best in binary class)/value
    # calculated_efficiency = (value for best in selected list of designs)/value
    # all efficiencies for a disconnected design are zero
    element phi_0 {
        # sum of log(z_i)
        element value { d | q | z | not_applicable} ,
        element absolute_efficiency { d | q | z | unknown } ? ,
        element calculated_efficiency { d | q | z | unknown } ?
    } ?
```

```
element phi_1 {
        # mean of the z_i
        element value { d | q | z | not_applicable} ,
        element absolute_efficiency { d | q | z | unknown } ? ,
        element calculated_efficiency { d | q | z | unknown } ?
    } ?
    element phi_2 {
        # mean of squared z_i
        element value { d | q | z | not_applicable} ,
        element absolute_efficiency { d | q | z | unknown } ? ,
        element calculated_efficiency { d | q | z | unknown } ?
    } ?
    element maximum_pairwise_variances {
        # largest of the v_{ij}
        element value { d | q | z | not_applicable} ,
        element absolute_efficiency { d | q | z | unknown } ? ,
        element calculated_efficiency { d | q | z | unknown } ?
    } ?
    element E_criteria {
        # cumulative sums of the z_i
        # E_1=z_1 is often called "the" E-value
        # E_2=z_1+z_2
        # E_3=z_1+z_2+z_3
        # etc
        # E_{v-1}=(v-1)*phi_1
        # Maximize all v-1 E-values <=> Schur-optimal
        E_value +
    } ?
}
E_value = element E_value {
    attribute index { xsd:positiveInteger } ,
    # index must be in \{1, \ldots, v-1\}
    element value { d | q | z | not_applicable} ,
    element absolute_efficiency { d | q | z | unknown } ? ,
    element calculated_efficiency { d | q | z | unknown } ?
}
other_ordering_criteria = element other_ordering_criteria {
    # these are criteria that order designs within the reference
    # universe but which do not meet our definition for
    # an "optimality" criterion
```

```
# may be of interest in conjunction with formal optimality criteria
    # in a multi-criterion screening of designs
   # absolute_comparisons and calculated_comparisons are handled just
    # as the corresponding efficiencies for optimality criteria (and in
    # particular are zero for every disconnected design); because they do
    # not measure relative size of a variance, we use a different terminology
    # all disconnected designs are ordered "last"
    element trace_of_square_of_C {
        # sum of z_i^{-2} = trace of C<sup>2</sup>
        # this is sometimes called the "S" criterion and is the second
        # stage of the "M-S" optimality search (first stage is to
 restrict to binarity, which maximizes trace)
#
        element value { d | q | z | not_applicable} ,
        element absolute_comparison { d | q | z | unknown } ? ,
        element calculated_comparison { d | q | z | unknown } ?
   } ?
    element max_min_ratio_canonical_variances {
        # z_1/z_{v-1}
        element value { d | q | z | not_applicable} ,
        element absolute_comparison { d | q | z | unknown } ? ,
        element calculated_comparison { d | q | z | unknown } ?
    } ?
    element max_min_ratio_pairwise_variances {
        # max(v_{ij})/min(v_{ij})
        element value { d | q | z | not_applicable} ,
        element absolute_comparison { d | q | z | unknown } ? ,
        element calculated_comparison { d | q | z | unknown } ?
    } ?
    element no_distinct_canonical_variances {
        # number of distinct values among the z_{i}
        element value { z | unknown | not_applicable } ,
        element absolute_comparison { d | q | z | unknown } ?
        element calculated_comparison { d | q | z | unknown } ?
    } ?
    element no_distinct_pairwise_variances {
        # number of distinct values among the v_{ij}
        element value { z | unknown | not_applicable } ,
        element absolute_comparison { d | q | z | unknown } ? ,
        element calculated_comparison { d | q | z | unknown } ?
    } ?
} ?
```

```
canonical_efficiency_factors = element canonical_efficiency_factors {
    attribute no_distinct { xsd:positiveInteger | "unknown" | "not_applicable" } ,
    # no_distinct = "not_applicable" for disconnected designs
    attribute ordered { "true" | "unknown" } ,
    element value {
       attribute multiplicity { xsd:positiveInteger | "not_applicable" } ,
        (d | q | z | blank)
    } +
    # for a design with u connected components, there must be u-1 values
    # of 0
}
functions_of_efficiency_factors = element functions_of_efficiency_factors {
    # These are functions of the canonical efficiency factors
   #
                  e_1 <= e_2 <= ... <= e_{v-1}
   # that "good" designs will maximize over the class of all designs
   # with the same blocksize distribution and fixed replication numbers
   # NOTE WELL: The reference universe for these functions is restricted
    # to designs with fixed v, block size distribution, AND replication
    # numbers!
    element harmonic_mean {
       attribute alias { "A" } ,
        element value { d \mid q \mid z }
    } ?
    element geometric_mean {
        attribute alias {"D"} ,
        element value { d \mid q \mid z }
    } ?
    element minimum {
        attribute alias { "E" } ,
        element value { d | q | z }
   } ?
}
robustness_properties = element robustness_properties {
    # for connected designs only
   robust_connected_plots ? ,
   robust_connected_blocks ? ,
   robust_efficiencies_plots ?
   robust_efficiencies_blocks ?
} ?
```

```
robust_connected_plots = element robust_connected_plots {
    # This element makes the statement
   # "The design is connected under all possible ways in which
   # number_lost plots can be removed"
   # If the reported value of number_lost is known to be the largest integer
   # for which this statement is true then is_max takes the value "true"
   # and otherwise takes the value "unknown."
   attribute number_lost { xsd:nonNegativeInteger } ,
   attribute is_max { "true" | "unknown" }
}
robust_connected_blocks = element robust_connected_blocks {
    # This element makes the statement
   # "The design is connected under all possible ways in which
   #
      number_lost blocks can be removed"
   # If the reported value of number_lost is known to be the largest integer
   # for which this statement is true then is max takes the value "true"
   # and otherwise takes the value ""unknown"."
   attribute number_lost { xsd:nonNegativeInteger } ,
                           { "true" | "unknown" }
   attribute is_max
}
robust_efficiencies_plots = element robust_efficiencies_plots {
   attribute precision
                          { xsd:positiveInteger } ,
   robustness_efficiency_values +
}
robust_efficiencies_blocks = element robust_efficiencies_blocks {
   attribute precision
                           { xsd:positiveInteger } ,
   robustness_efficiency_values +
}
robustness_efficiency_values = element robustness_efficiency_values {
   # n=0 not allowed for number_lost
   # self_efficiency =
                             (value of the criterion for the full design)/
                              (value for the reduced design)
   #
   # absolute_efficiency = (value for best in reduced binary class)/
                              (value for the reduced design)
   #
   # calculated_efficiency = (value for best in selected list of designs)/
   #
                              (value for the reduced design)
   attribute number_lost { xsd:positiveInteger } ,
   attribute loss_measure { "average" | "worst" } ,
    element phi_0 {
       # sum of log(z_i)
       element self_efficiency
                                {d|q|z},
```

```
element absolute_efficiency { d | q | z | unknown } ? ,
       element calculated_efficiency { d | q | z | unknown } ?
   } ?
   element phi_1 {
       # mean of the z_i
       element self_efficiency
                                 {d|q|z},
       element absolute_efficiency { d | q | z | unknown } ? ,
       element calculated_efficiency { d | q | z | unknown } ?
   } ?
   element maximum_pairwise_variances {
       # largest of the v_{ij}
       element self_efficiency
                                     {d|q|z},
       element absolute_efficiency { d | q | z | unknown } ? ,
       element calculated_efficiency { d | q | z | unknown } ?
   } ?
   element E_1 {
       # E_1=z_1 is often called "the" E-value
       element self_efficiency \{ d \mid q \mid z \},
       element absolute_efficiency { d | q | z | unknown } ? ,
       element calculated_efficiency { d | q | z | unknown } ?
   } ?
}
alternative_representations = element alternative_representations {
   incidence_matrix
   # ... to be extended as needed
}
incidence_matrix = element incidence_matrix {
   attribute shape { "points_by_blocks" } ,
   matrix
}
# latin square
# (place holder only, to be defined later)
latin_square = element latin_square { empty }
# vi: set syntax=rnc:
# vi: set expandtab:
```

# B An example

Here in its entirety is the example which we have seen in parts throughout this document.

```
<?xml version="1.0"?>
<list_of_designs design_type="block_design" dtrs_protocol="1.1" no_designs="1"</pre>
pairwise_nonisomorphic="true" xmlns="http://designtheory.org/xml-namespace">
    <block_design b="7" id="t2-v7-k3-L1-1" v="7">
        <blocks ordered="true">
            <block><z>0</z><z>1</z><z>2</z></block>
            <block><z>0</z><z>3</z><z>4</z></block>
            <block><z>0</z><z>5</z><z>6</z></block>
            <block><z>1</z><z>3</z><z>5</z></block>
            <block><z>1</z><z>4</z><z>6</z></block>
            <block><z>2</z><z>3</z><z>6</z></block>
            <block><z>2</z><z>4</z><z>5</z></block>
        </blocks>
        <indicators>
            <repeated_blocks flag="false">
            </repeated_blocks>
            <resolvable flag="false">
            </resolvable>
            <affine_resolvable flag="false">
            </affine_resolvable>
            <equireplicate flag="true" r="3">
            </equireplicate>
            <constant_blocksize flag="true" k="3">
            </constant_blocksize>
            <t_design flag="true" maximum_t="2">
            </t_design>
            <connected flag="true" no_components="1">
            </connected>
            <pairwise_balanced flag="true" lambda="1">
            </pairwise_balanced>
            <variance_balanced flag="true">
            </variance_balanced>
            <efficiency_balanced flag="true">
            </efficiency_balanced>
            <cyclic flag="true">
            </cyclic>
            <one_rotational flag="false">
            </one_rotational>
        </indicators>
```

```
<combinatorial_properties>
    <point_concurrences>
        <function_on_ksubsets_of_indices domain_base="points" k="1"
         n="7" ordered="true" title="replication_numbers">
            <map>
                <preimage>
                    <entire_domain>
                    </entire_domain>
                </preimage>
                <image><z>3</z></image>
            </map>
        </function_on_ksubsets_of_indices>
        <function_on_ksubsets_of_indices domain_base="points" k="2"
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