# Stabilization Algorithms for Configurations

Sven Reichard

TU Dresden

<2018-07-02 Mo>

### Outline

#### Basics

#### Binary coherent configurations

Generalization

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### Numbers, Tuples

- ► We identify the natural number n with the set {0,..., n − 1} of all smaller numbers.
- If we want to emphasize the "setness" we will write [n] instead of n.
- Tuples over a set  $\Omega$  are functions  $x:[n] \rightarrow \Omega$
- As usual we denote the set of all function from A to B by B<sup>A</sup>.

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▶ In particular, the set of all n-tuples of B is B<sup>[n]</sup>=B<sup>n</sup>.

### Kernels, equivalence relations



• Given  $f : A \rightarrow B$ , its kernel is the relation

ker 
$$f = \{(x, y) \in A^2 \mid f(x) = f(y)\}.$$

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This is an equivalence relation.

#### Tuples and permutations

- By S(A) we denote the symmetric group of all permutations of
  A. Since permutations are functions they act on the left.
- ▶ If  $x \in A^n$  and  $\sigma \in S([n])$ , then  $x \circ \sigma$  is the permuted tuple:  $(x \circ \sigma)(i) = x_{\sigma(i)}$ .
- If x is as above, and φ ∈ S(A), then φ ∘ x is the coordinatewise image of x under φ:

$$(\varphi \circ x)(i) = \varphi(x_i).$$

So,

$$\varphi \circ x = (\varphi(x_0), \ldots, \varphi(x_{n-1})).$$

# Refinement of functions

- For functions f : A → B, g : A → C, we say f ≤ g if ker f ⊆ ker g. In the case of equality we write f~ g. If B = C we get a quasiorder on B<sup>A</sup>
- If B is at most countable, then for any f:A→ B there is a g : A → N with f~ g. So below we can restrict ourselves to functions with codomain N
- So we may translate between functions, equivalence relations and partitions

Binary coherent configurations

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#### Introduction

- We recall the definition and motivation of coherent configurations.
- ► Later we will formalize and generalize these notions.

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### Colorings

A k-coloring of Ω is a function

$$r: \Omega^k \to C$$

that assigns to each k-tuple in  $\Omega$  a color from a set C.

- For k = 2 we think of a coloring of the edges of the complete graph on  $\Omega$ .
- For now we look at the binary case and recall the notion of coherent configurations.

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# Binary configurations

- A binary coloring r of Ω is a configuration if the following properties hold:
  - 1. Reflexive pairs and irreflexive pairs do not share colors;

- 2. If r(x, y) = r(x', y'), then r(y, x) = r(y', x').
- Some people refer to configurations as rainbows.

# Different languages

- Given a binary coloring r the preimage of each color is a binary relation on  $\Omega$ .
- $\blacktriangleright$  Hence a coloring defines a set of binary relations on  $\Omega$  such that  $\Omega^2$  is its disjoint union.
- Conversely, any such system of relations defines a coloring.

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# Configurations as systems of relations

- In these terms we can define binary configurations as follows:
- A set S of binary relations on  $\Omega$  is a configuration if
  - each relation is reflexive or irreflexive
  - if  $s \in S$  then  $s^* \in S$ .
- Here,  $s^* = \{(y, x) \mid (x, y) \in s\}$  is the inverse of s.
- We will switch freely between the languages of colorings and relations

# 2-homogeneous configurations

- Let G be a group acting on Ω
- The orbits of G on  $\Omega^2$  form a configuration
- We say that a configuration is 2-homogeneous if it "comes from a group"
- More formally it means that the automorphism group acts transitively on each of the relations (better definition will follow)

# Example: $C_6$

#### • Define the following configuration on $\Omega = Z_6$ :

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$$R_0 = \{(\mathbf{x}, \mathbf{x}) | \mathbf{x} \in \Omega \}$$

$$R_1 = \{(x,y) | x - y \in \{1,5\}\}$$

$$\blacktriangleright R_2 = \Omega^2 \setminus (R_0 \cup R_1)$$

- This is a configuration.
- Does it come from a group?

#### Invariants

- Given a configuration we may define invariants on pairs of points.
- For example, we can count triangles of given given colors
  Given (x,y)∈ Ω<sup>2</sup> and colors i,j, we count

$$\{z \in \Omega \mid r(x,z) = i, r(z,y) = j\}$$

In the C<sub>6</sub> example this allows us to distinguish long and short diagonals

### Stabilization

- Such invariants can be used to refine the given coloring
- Configurations stable under this refinement are called *coherent*

- 2-homogeneous configurations are always coherent
- The converse does not hold.

# Weisfeiler-Leman

- Each coloring has a unique "smallest" coherent refinement
- We call it the coherent closure
- This is in turn refined by the 2-orbits of the automorphism group
- So we get a "combinatorial approximation" of the automorphism group
- The coherent closure can be computed in polynomial time, this was first described by Weisfeiler and Leman
- Several practical implementations were described by Babel, Chuvaeva, Klin, Pasechnik in the 1990's
- We might see an example of such calculations at the end of the presentation

### General configurations

- We generalize the notion of coherent configurations in several aspects:
  - Instead of binary configurations we consider arbitrary arity
  - Instead of triangles we count substructures of arbitrary size.

- It is often convenient to use the language of colorings
- But what are useful generalizations of the axioms of configurations?

- We look at the defining properties of binary configurations and coherent configurations one by one
- We try to give "natural" generalizations for colorings of higher arity
- ▶ This will lead objects similar to systems of *k*-orbits of groups.

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# Reflexive/irreflexive

The first property of binary configurations states that reflexive and irreflexive pairs have different colors

- Irreflexive pairs have a discrete kernel; reflexive pairs have a trivial kernel
- So the first condition for a k-ary coloring r is:

• If 
$$r(x) = r(y)$$
, then  $\ker(x) = \ker(y)$ .

#### Inverses

- The second property was: If two pairs have the same color, then the reverse pairs also have the same color
- For k-tuples we can apply arbitrary permutations:
  - If r(x) = r(y), and  $\sigma \in S_k$ , then  $r(x \circ \sigma) = r(y \circ \sigma)$

### k-ary configurations

• Let  $r: \Omega^k \to C$  be a k-coloring.

We call r a k-ary configuration if the following conditions hold:

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For 
$$x, y \in \Omega^k$$
:  $r(x) = r(y) \Longrightarrow \ker(x) = \ker(y)$   
For  $\sigma \in S_k$ , if  $r(x) = r(y)$  then  $r(x \circ \sigma) = r(y \circ \sigma)$ .

We call |Ω| the order of r; k its arity, and the cardinality |r (Ω<sup>k</sup>)| of its image the rank of r.

# Group configurations

- Let G be a group acting on  $\Omega$ .
- For  $x \in \Omega^k$  and  $g \in G$  we have  $g \circ x \in \Omega^k$ .
- This defines an action of G on  $\Omega^k$ .
- The orbits of this action form a k-ary configuration  $(G,\Omega)^k$

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For now we call these group configurations

# Subconfigurations

- Let r be a k-ary coloring on Ω
- Let  $x \in \Omega^m$  be a tuple
- Let  $x^k : [m]^k \to \Omega^k$  be the k-fold tupling of x
- ► Then r ∘ x<sup>k</sup> is a k-ary coloring of [m], the coloring r<sub>x</sub> induced by x.

#### Lemma

If r is a configuration and x is one-to-one then  $r_x$  is a configuration.

#### Homomorphisms

- Let  $W_1 = (\Omega_1, C_1, r_1)$  and  $W_2(\Omega_2, C_2, r_2)$  be k-ary structures. Let  $\varphi : \Omega_1 \to \Omega_2$  be a function.
  - $\varphi$  is a weak homomorphism if for any  $x, y \in \Omega_1^k$  we have  $r_1(x) = r_1(y) \Longrightarrow r_2(\varphi(x)) = r_2(\varphi(y))$ . We write  $\varphi : W_1 \to W_2$ .

•  $\varphi$  is a strong homomorphism if  $r_2 \circ \varphi = r_1$ .

A bijective strong homomorphism is an isomorphism

### Homogeneity

- Let r be a k-ary configuration.
- If every isomorphism between subconfigurations of order at most m extends to an automorphism, we say that r is m-homogeneous.
- More formally: r is m-homogeneous if for any  $x, y \in \Omega^m$  with  $r_x = r_y$  there is an automorphism  $\sigma$  of r with

$$y = x \circ \sigma$$

#### Lemma

W is k-homogeneous iff it is a group configuration.

#### Extensions of vectors

Let n ≥ m, x ∈ A<sup>m</sup>, y ∈ A<sup>n</sup>. We call y an n-extension of x if they coincide on the first m coordinates, i.e., x = y|<sub>[m]</sub>.

Denote the set of all extensions of x by

$$A_x^n = \{y \in A^n \mid y|_{[m]} = x\}$$

We denote multisets by using square brackets. E.g.,

$$[x^2 | x \in \mathbb{Z}, -2 \le x \le 2] = [0, 1, 1, 4, 4].$$

# (m,t)-invariant

• Let  $W = (\Omega, C, r)$  be a k-ary configuration.

• Let 
$$t \ge m \ge k$$
, let  $x \in \Omega^m$ .

We consider the multiset of configurations induced by all t-extensions of x.

$$W_x^t = [W_y \mid y \in \Omega_x^t]$$

#### Lemma

This invariant can be computed in polynomial time.

# (m,t)-coherent configurations

#### We say that W is (m, t)-coherent if it is stable under this invariant.

# Lemma If $m' \leq m$ and $t' \leq t$ then any (m, t)-coherent configuration is (m', t')-coherent.

# (k,t)-coherent closure

- Any k-ary configuration has a unique smallest (k,t)-coherent closure.
- This closure can be computed in time  $n^{O(t)}$ .
- This constitutes a Schurian polynomial approximation scheme in the sense of Evdokimov-Ponomarenko, 1999

# Connection to other notions of regularity

#### Lemma

A k-ary configuration is coherent if and only if it is (k, k + 1)-coherent.

- In particular, classical (binary) coherent configurations are precisely (2,3)-coherent.
- Hestenes and Higman introduced the t-vertex condition for graphs to get a stronger combinatorial characterization of rank 3 groups

#### Lemma

A binary configuration satisfies the t-vertex condition if and only if it is (2, t)-coherent.

#### Lemma

A k-ary configuration of order n is m-homogeneous if and only if it is (m, n)-coherent.

So we have a family of properties for k-ary configurations which subsumes several regularity conditions considered earlier.

#### Implementation

- We have an implementation that computes (m,t)-coherent closures
- It still needs some optimization
- However it is a working program for this general problem
- The code will be available at
  - http://www.github.com/sven-reichard/stabilization

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#### Demonstration

Classical WL-Stabilization for Möbius ladders

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(2,4)-stabilization of Shrikhande's graph

#### Main question

Are there (m,t)-coherent configurations which are not m-homogeneous, for large values of m and/or t?

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- If yes, these should be rare and interesting objects.
- If not, we have solved the isomorphism problem

### A related notion and examples

- Pech has introduced a similar notion for simple graphs
- His concept corresponds to (m,t)-coherence of binary configurations with three colors.
- He gives examples of (3,7)-coherent graphs arising from generalized quadrangles.

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