

# Relational Colour Refinement for Non-Relational Signatures

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- Colour Refinement is an important and interesting algorithm
- Applied in modern isomorphism solvers
- Can be characterised logically and combinatorially
- Extension to more than graphs seems desirable
- Scheidt and Schweikardt, 2025 introduced Relational Colour Refinement
- Conceptually similar to classical Colour Refinement
- Also has a logical and a combinatorial characterisation

# Contents of this presentation

1. Classical Colour Refinement
2. Relational Colour Refinement
3. Relational Colour Refinement for Structures With Functions
4. Restricting RCR to Subclasses of Relational Structures
5. Conclusion

# Classical Colour Refinement

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- Also called *CR* or *1-dimensional Weisfeiler-Leman* algorithm
- Iterative graph algorithm
- Constructs colour for every vertex, based on colours of neighbours
- Initial colour for every  $v \in V$ :  $C_0(v) = 0$
- Next rounds:  $C_{i+1}(v) := (C_i(v), \{ \{ C_i(u) : \{v, u\} \in E \} \})$
- CR distinguishes two graphs  $G$  and  $H$ , if
  - there exists  $C_i(v)$  in colouring of  $G$  or  $H$ , such that the number of vertices with colour  $C_i(v)$  is different in  $G$  than in  $H$

- There are equivalent characterisations for CR
- Logical characterisation:  
CR distinguishes  $G$  and  $H$  if, and only if, there exists  $\varphi \in \mathcal{C}_2$ , such that  $G \models \varphi$  and  $H \not\models \varphi$
- Combinatorial characterisation:  
CR distinguishes  $G$  and  $H$  if, and only if, there exists tree  $T$ , such that  $\text{hom}(T, G) \neq \text{hom}(T, H)$

## Relational Colour Refinement

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# Relational Colour Refinement (RCR)

- Applies variant of classical Colour Refinement on tuples of structure
- Uses set of relations that contain tuple as part of initial colouring
- Uses pairs of indices as edges to mark shared elements of tuples
- Formally:

$$\text{atp}(\mathbf{a}) = \{R \in \sigma : \mathbf{a} \in R\}$$

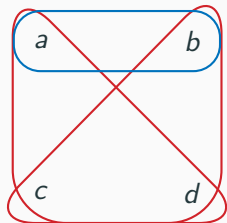
and

$$\text{stp}(\mathbf{a}, \mathbf{b}) = \{(i, j) \in [n] \times [m] : \mathbf{a}_i = \mathbf{b}_j\}$$

- For relational structure  $\mathfrak{A}$  and all tuples  $\mathbf{a} \in \bigcup_{R \in \sigma} R^{\mathfrak{A}}$ :
  - Initial colour:  $\varrho_0(\mathbf{a}) = (\text{atp}(\mathbf{a}), \text{stp}(\mathbf{a}, \mathbf{a}))$
  - For the next rounds:  $\varrho_{i+1}(\mathbf{a}) = (\varrho_i(\mathbf{a}), \{\{(\text{stp}(\mathbf{a}, \mathbf{b}), \varrho_i(\mathbf{b})) : \text{stp}(\mathbf{a}, \mathbf{b}) \neq \emptyset\}\})$



# An Example for RCR

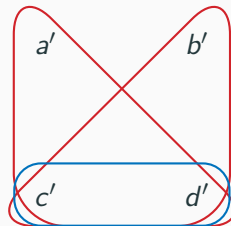
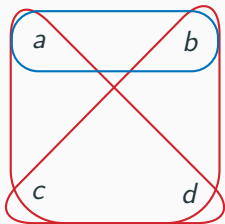


- Structure  $\mathfrak{A} = (A, R^{\mathfrak{A}}, T^{\mathfrak{A}})$

- $\varrho_0((a, b)) = (\{R\}, \{(1, 1), (2, 2)\})$  and  
 $\varrho_0((a, c, d)) = \varrho_0((b, c, d)) = (\{T\}, \{(1, 1), (2, 2), (3, 3)\})$
- $\varrho_1((a, c, d)) = (\varrho_0((a, c, d)), \{\{ \{(1, 1)\}, \varrho_0((a, b)) \}, \dots \})$  and  
 $\varrho_1((b, c, d)) = (\varrho_0((b, c, d)), \{\{ \{(1, 2)\}, \varrho_0((a, b)) \}, \dots \})$

# Distinguishing Relational Structures with RCR

- RCR distinguishes, if some colour appears differently often in the structures



- $\varrho_1((a, c, d))$  appears in colouring of left structure but not in right

# Guarded Fragment of Counting Logic

- $C_2$  characterises CR on graphs
- Guarded fragment of counting logic  $GF(C)$  characterises RCR

## Guarded Fragment of Counting Logic

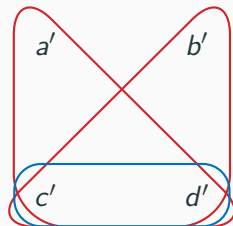
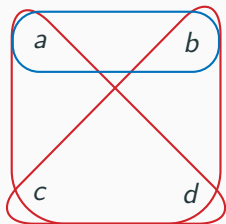
- Everything except for quantifiers defined as in classical counting logic
- For atomic formula  $\Delta \in GF(C)$  and formula  $\varphi \in GF(C)$ , we call  $\Delta$  a guard for  $\varphi$ , if  $\text{free}(\Delta) \supseteq \text{free}(\varphi)$
- Quantifiers appear only in form  $\exists^{\geq i} \mathbf{v} . (\Delta \wedge \varphi)$ , where  $\Delta$  is guard for  $\varphi$  and  $\text{set}(\mathbf{v}) \subseteq \text{free}(\Delta)$
- Examples:
  - $\exists^{\geq 2}(x, y) . (E(x, y) \wedge T(y)) \in GF(C)$
  - $\exists^{\geq 3}(x, y, z) . (E(x, y) \wedge E(y, z) \wedge E(z, x)) \notin GF(C)$

## Theorem B (Scheidt and Schweikardt, 2025)

Let  $\mathfrak{A}$  and  $\mathfrak{B}$  be two relational structures. Then the two following statements are equivalent.

1. RCR distinguishes  $\mathfrak{A}$  and  $\mathfrak{B}$
2. There exists a sentence in  $\text{GF}(\text{C})$  that is satisfied by  $\mathfrak{A}$ , but not by  $\mathfrak{B}$

## Example for Logical Characterisation of RCR



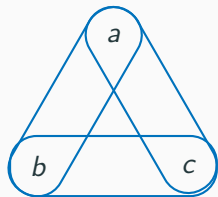
- We have seen RCR distinguishes the structures
- Formula  $\exists^{\geq 1}(x, y, z). (T(x, y, z) \wedge \exists^{\geq 1}(y). (R(x, y)))$  satisfied by left and not by right structure

- Counting homomorphisms from trees characterises CR on graphs
- Abstraction from trees to relational structures is needed:  $\alpha$ -acyclic structures (in the following only acyclic structures)

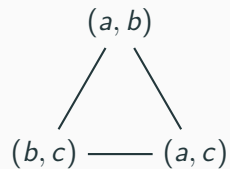
## Acyclic Structures

- Relational structure  $\mathcal{C}$  is acyclic if it has a join tree  $J$
- Join tree  $J$  is tree with  $V(J) = \bigcup_{R \in \sigma} R^{\mathcal{C}}$  and fulfils join-tree-property:
  - For every  $e \in C$ , the set  $\{\mathbf{x} \in V(J) : e \in \text{set}(\mathbf{x})\}$  induces a connected subtree

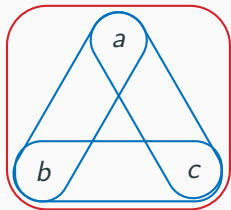
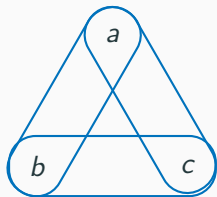
## Examples for Acyclic Structures



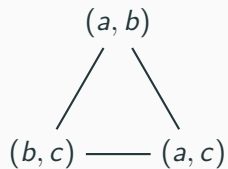
No:



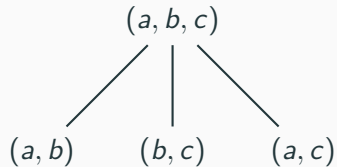
## Examples for Acyclic Structures



No:



Yes:



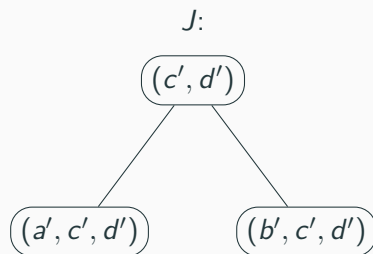
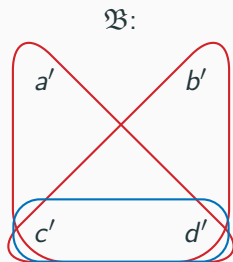
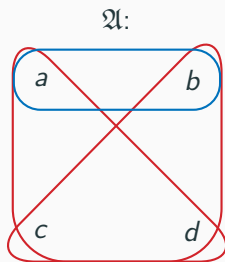


## Theorem A (Scheidt and Schweikardt, 2025)

Let  $\mathfrak{A}$  and  $\mathfrak{B}$  be relational structures. Then the two following statements are equivalent.

1. RCR distinguishes  $\mathfrak{A}$  and  $\mathfrak{B}$
2. There exists an acyclic relational structure  $\mathfrak{C}$ , such that it distinguishes  $\mathfrak{A}$  and  $\mathfrak{B}$  by homomorphism count

## Example for Combinatorial Characterisation of RCR



- $J$  is join tree for  $\mathfrak{B}$ , therefore  $\mathfrak{B}$  is acyclic
- Identity is homomorphism, so  $\mathfrak{B}$  has at least one homomorphism to itself
- $\mathfrak{B}$  has no homomorphisms to  $\mathfrak{A}$

# Relational Colour Refinement for Structures With Functions

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- Many interesting structures use functions
- Colour Refinement algorithm for such structures seems desirable
- Will use the results of Scheidt and Schweikardt and investigate how robust they are
- Following structure:
  1. Presentation of two approaches for Colour Refinement for non-relational signatures
  2. Logical characterisation of both approaches
  3. Discussion on combinatorial characterisation

- Goal: Encode non-relational structures and signatures as relational ones
- Functions can directly be interpreted as relations:

$$f(\mathbf{x}) = y \iff (\mathbf{x}y) \in R_f$$

- For non-relational signature  $\sigma$  define relational signature  $\sigma'$ :
  - Inherit relation symbols from  $\sigma$
  - Function symbol  $f \in \sigma$  of arity  $n \rightarrow$  introduce  $R_f \in \sigma'$  of arity  $n + 1$
- Encode  $\sigma$ -structure  $\mathfrak{A}$  as  $\sigma'$ -structure  $\mathfrak{A}'$ :
  - Relations like in  $\mathfrak{A}$
  - For function symbol  $f \in \sigma$ :  $R_f^{\mathfrak{A}'} := \{(\mathbf{x}y) : f^{\mathfrak{A}}(\mathbf{x}) = y\}$
- We say *naive RCR* distinguishes  $\mathfrak{A}$  and  $\mathfrak{B}$ , if RCR distinguishes the encodings

## Idea of the Transitive Expansion

- Approach is only defined for unary function symbols
- Encoding emulates the nesting of function applications
- Encode function  $f$  as family of relations  $R_{f^1}, R_{f^2}, \dots$ , where  $(x, y) \in R_{f^i}$  if  $\underbrace{f(f(\dots f(x)))}_{i \text{ times}} = y$
- In the following:  $f^i(x)$  written for  $\underbrace{f(f(\dots f(x)))}_{i \text{ times}}$
- For multiple functions, also encode alternations, for example  $R_{fg}$  or  $R_{g^2f^3}$

## Alternations of Function Applications

- Let  $\sigma$  be signature with unary function symbols
- Define set of all allowed function application alternations  $\text{Alters}_n^k(\sigma)$  as all sequences of up to  $k$  function symbols, where
  1. Every function symbol has exponent in  $[n]$
  2. Two succeeding function symbols are different

- Example:

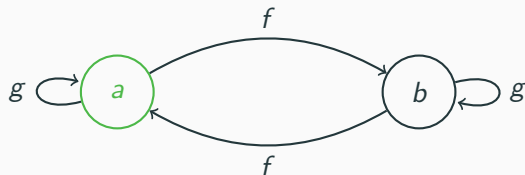
$$\begin{aligned} & \circ \sigma = \{f/1, g/1\} \\ & \circ \text{Alters}_2^2(\sigma) = \underbrace{\{\text{id}\}}_{k=0} \cup \underbrace{\{f, f^2, g, g^2\}}_{k=1} \cup \underbrace{\{fg, fg^2, f^2g, f^2g^2, gf, \dots\}}_{k=2} \end{aligned}$$

## Transitive Expansion

- For alternation depth  $k$  and  $\sigma$ -structure  $\mathfrak{A}$  with  $|\mathfrak{A}| = n$  define signature  $\tilde{\sigma}$  and transitive expansion  $\tilde{\mathfrak{A}}$  as  $\tilde{\sigma}$ -structure
- For all  $\alpha, \beta, \alpha_1, \dots, \alpha_\ell \in \text{Alters}_n^k(\sigma)$  and relation symbol  $R \in \sigma$  of arity  $\ell$ , insert relation symbol  $\text{Eq}_{\alpha, \beta}$  of arity 2 and relation symbol  $R_{\alpha_1, \dots, \alpha_\ell}$  of arity  $\ell$  into  $\tilde{\sigma}$
- Define  $\text{Eq}_{\alpha, \beta}^{\tilde{\mathfrak{A}}} := \{(x, y) : \alpha^{\mathfrak{A}}(x) = \beta^{\mathfrak{A}}(y)\}$  and  $R_{\alpha_1, \dots, \alpha_\ell}^{\tilde{\mathfrak{A}}} := \{(x_1, \dots, x_\ell) : (\alpha_1^{\mathfrak{A}}(x_1), \dots, \alpha_\ell^{\mathfrak{A}}(x_\ell)) \in R^{\mathfrak{A}}\}$
- For  $k \in \mathbb{N}$  we say that  $\text{RCR}_k$  distinguishes structures  $\mathfrak{A}$  and  $\mathfrak{B}$ , if  $\text{RCR}$  distinguishes the transitive expansions with alternation depth  $k$

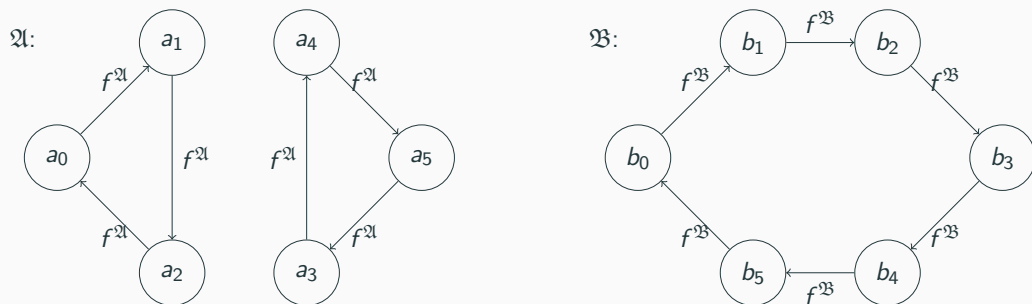


## Example for the Transitive Expansion



- Structure  $\mathfrak{A} = (A, \mathbf{R}^{\mathfrak{A}}, f^{\mathfrak{A}}, g^{\mathfrak{A}})$
- $k = 1$  and  $n = 2$ :  $\text{Alters}_2^1(\sigma) = \{\text{id}, f, f^2, g, g^2\}$
- $\tilde{\sigma} = \{R_{\text{id}}, R_f, R_{f^2}, R_g, R_{g^2}, \text{Eq}_{\text{id}, \text{id}}, \text{Eq}_{\text{id}, f}, \text{Eq}_{\text{id}, f^2}, \dots, \text{Eq}_{g^2, g^2}\}$
- Examples:
  - $R_f^{\tilde{\mathfrak{A}}} = \{b\}$
  - $\text{Eq}_{f^2, \text{id}}^{\tilde{\mathfrak{A}}} = \{(a, a), (b, b)\}$
  - $\text{Eq}_{g, f}^{\tilde{\mathfrak{A}}} = \{(a, b), (b, a)\}$

# Naive Encoding versus Transitive Expansion



- Cannot be distinguished by naive RCR: Encodings result in regular graphs
- But: Distinguished by Transitive Expansion Encoding
  - We find that  $\text{Eq}_{f^1, \text{id}}^{\mathfrak{A}} = \text{Eq}_{f^4, \text{id}}^{\mathfrak{A}}$ , not for  $\mathfrak{B}$
  - Sentence  $\exists^{\geq 6}(x, y) \cdot (\text{Eq}_{f^1, \text{id}}(x, y) \wedge \text{Eq}_{f^4, \text{id}}(x, y)) \in \text{GF}(\mathbb{C})$  distinguishes encodings

# **Relational Colour Refinement for Structures With Functions**

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**Logical Characterisations for Both Approaches**

## Nesting-Free Guarded Fragment of Counting Logic

- Extends given definition of  $\text{GF}(\text{C})$  for non-relational signatures
- Allow atomics of the following forms
  - Relation symbols and variable equations like in  $\text{GF}(\text{C})$
  - For function symbol  $f$  of arity  $\ell$  and variables  $x_1, \dots, x_\ell, y$ :  
$$f(x_1, \dots, x_\ell) = y \in \text{nfGF}(\text{C})$$
- Forbid nesting of terms, for example  $f(g(x), y) = z$
- Informally: Usage of function symbols like relation symbols

## Logical Characterisation of Naive RCR

Let  $\mathfrak{A}$  and  $\mathfrak{B}$  be structures.

Naive RCR distinguishes  $\mathfrak{A}$  and  $\mathfrak{B}$   
iff.

There exists a sentence  $\varphi \in \text{nfGF}(\mathcal{C})$  which is fulfilled by  $\mathfrak{A}$ , but not by  $\mathfrak{B}$

*Proof idea:*

- Naive RCR distinguishes structures iff. RCR distinguishes encodings iff. there exists a sentence in  $\text{GF}(\mathcal{C})$  that distinguishes the encodings
- Define translation of  $\text{GF}(\mathcal{C})$  to and from  $\text{nfGF}(\mathcal{C})$ 
  - Replace  $R_f(\mathbf{x}y)$  by  $f(\mathbf{x}) = y$

## GF(C) with alternation depth $k$ ( $\text{GF}(C)_k$ )

### GF(C) with alternation depth $k$

- Fixate  $k \in \mathbb{N}$
- Atomics are defined like in natural extension to non-relational signatures, with one restriction
- For every formula in  $\text{GF}(C)_k$  and every term  $t$  that appears in it, there must exist a  $n \in \mathbb{N}$ , such that  $t = \alpha$  for a  $\alpha \in \text{Alters}_n^k(\sigma)$
- Restrict number of alternations of function applications to  $k$
- No restriction of number of application of same function in series
- Examples:
  - $f^2(g(h^3(x))) = y \notin \text{GF}(C)_2$ , but in  $\text{GF}(C)_3$
  - $f^i(x) = y \in \text{GF}(C)_1$  for all  $i \in \mathbb{N}$

## Logical Characterisation of $\text{RCR}_k$

Let  $k \in \mathbb{N}$  and let  $\mathfrak{A}$  and  $\mathfrak{B}$  be two structures.

$\text{RCR}_k$  distinguishes  $\mathfrak{A}$  and  $\mathfrak{B}$   
iff.

There exists a sentence in  $\text{GF}(\text{C})_k$  that is fulfilled by  $\mathfrak{A}$ , but not by  $\mathfrak{B}$

- 1. to 2.: Similar to before, translation from  $\text{GF}(\text{C})$  to  $\text{GF}(\text{C})_k$  very simple
- 2. to 1.: Assume  $n = |\mathfrak{A}| = |\mathfrak{B}|$ 
  - Translate and replace all atomic subformulae by formula that:
    - is equivalent for all structures with  $n$  elements
    - only contains terms  $f^i(s(x))$  with  $i \leq n$
  - Rearrange resulting formula to get valid  $\text{GF}(\text{C})_k$ -sentence
  - Results in equivalent formula for structures with  $n$  elements and for every term  $t$  there exists an  $\alpha \in \text{Alters}_n^k(\sigma)$ , such that  $t = \alpha$
  - Can easily be translated into sentence in  $\text{GF}(\text{C})$  of signature  $\tilde{\sigma}$

# **Relational Colour Refinement for Structures With Functions**

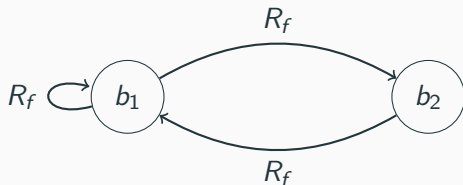
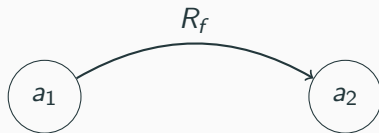
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**Discussion on the Combinatorial Characterisation**



# Total and Functional Structures

- Let  $\sigma$  be a signature,  $\sigma'$  its naive encoding and  $\mathfrak{A}'$  a  $\sigma'$ -structure
- We call  $\mathfrak{A}'$  total if for every function symbol  $f \in \sigma$  and every tuple  $\mathbf{x}$  there is a  $y$ , such that  $(\mathbf{x}y) \in R_f^{\mathfrak{A}'}$
- We call  $\mathfrak{A}'$  functional if for every function symbol  $f \in \sigma$  there are no two tuples  $(\mathbf{x}y), (\mathbf{x}z) \in R_f^{\mathfrak{A}'}$



- Will define acyclicity w.r.t. the naive encoding

## Non-Relational Acyclic Structures

- Let  $\mathfrak{A}$  be a non-relational structure
- We call  $\mathfrak{A}$  acyclic, if its naive encoding  $\mathfrak{A}'$  is acyclic

# Total and Functional Structures as Encodings

- Desired equivalence:

Non-relational, acyclic structure distinguishes  $\mathfrak{A}$  and  $\mathfrak{B}$  by homomorphism count  
?

Naive RCR distinguishes  $\mathfrak{A}$  and  $\mathfrak{B}$

- Result: Forward direction holds, backwards does not
- First step: Reformulate first statement:

Some non-relational, acyclic structure dist.  $\mathfrak{A}$  and  $\mathfrak{B}$  by hom. count  
iff.

Some total, functional and acyclic structure dist. encodings  $\mathfrak{A}'$  and  $\mathfrak{B}'$  by hom.  
count

- We can show:

Acyclic  $\sigma'$ -structure dist.  $\mathfrak{A}'$  and  $\mathfrak{B}'$  by hom. count  
iff.

Functional and acyclic  $\sigma'$ -structure dist.  $\mathfrak{A}'$  and  $\mathfrak{B}'$  by hom. count

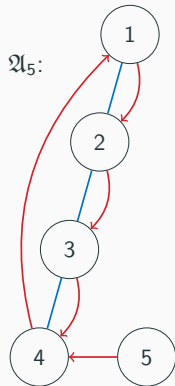
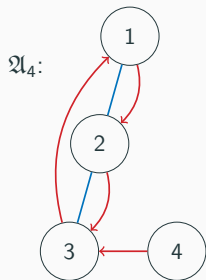
*Proof idea:*

- Backwards direction is obvious
- Forwards direction eliminates collisions of the form  $(xy), (xz) \in R_f$  by contracting  $y$  and  $z$
- This can be done while maintaining the homomorphisms and acyclicity and can be repeated until no collisions remain

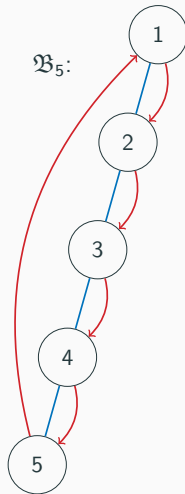
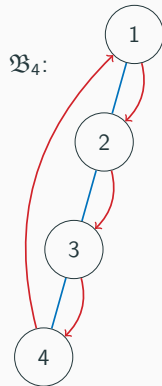
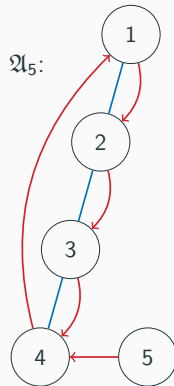
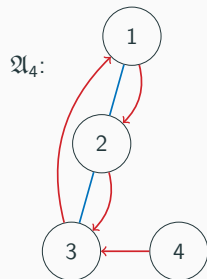
## Non-Enforceability of Totality

- There are structures that are distinguished by naive RCR, but there is no acyclic and total structure that distinguishes the encodings by homomorphism count
- Define signature  $\sigma = \{E/2, f/1\}$
- Two families of  $\sigma$ -structures  $(\mathfrak{A}_i)_{i \in \mathbb{N}_{\geq 4}}$  and  $(\mathfrak{B}_i)_{i \in \mathbb{N}_{\geq 4}}$
- For all  $i \in \mathbb{N}_{\geq 4}$ : Naive RCR distinguishes  $\mathfrak{A}_i$  and  $\mathfrak{B}_i$ , but no total and acyclic structure can distinguish the encodings by hom. count

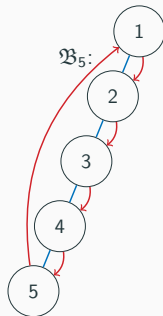
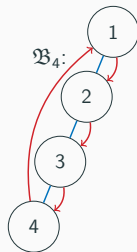
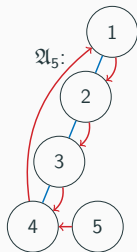
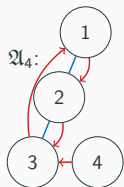
## Non-Enforceability of Totality ii



## Non-Enforceability of Totality ii



## Non-Enforceability of Totality iii



- Obviously distinguished by naive RCR
- If structure has  $R_f$ -loops or  $R_f$ -2-cycles, then no homomorphisms to either structure
- Because total, it has to contain larger  $R_f$ -cycles, but then cannot be acyclic



# Results of combinatorial characterisation of naive RCR

We have the following results:

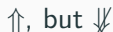
Naive RCR distinguishes  $\mathfrak{A}$  and  $\mathfrak{B}$



There exists acyclic structure that dist. encodings  $\mathfrak{A}'$  and  $\mathfrak{B}'$  by hom. count



There exists *functional* and acyclic structure that dist. encodings by hom. count



There exists *total*, functional and acyclic structure that dist. encodings by hom. count



There exists *non-relational* and acyclic structure that dist.  $\mathfrak{A}$  and  $\mathfrak{B}$  by hom. count

## Restricting RCR to Subclasses of Relational Structures

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- For what subclass  $\mathcal{S}$  of relational structures do we have the following equivalence:

Two structures from  $\mathcal{S}$  get distinguished by RCR  
iff.

There exists an acyclic structure from  $\mathcal{S}$  that dist. the structures by hom. count

- Does not hold for class of total structures
  - Encodings of families of structures from before are total, but no total and acyclic structure dist. them by hom. count
- Another class to investigate: Class of symmetric structures

## Restriction to Symmetric Structures

- Relational Structure is symmetric, if for every relation  $R$  and for every tuple  $\mathbf{x} \in R$ , every permutation of the elements in  $\mathbf{x}$  is also in  $R$

## Restriction to Symmetric Structures

- Relational Structure is symmetric, if for every relation  $R$  and for every tuple  $\mathbf{x} \in R$ , every permutation of the elements in  $\mathbf{x}$  is also in  $R$
- For two symmetric structures we can show

There exists acyclic structure that dist. the structures by hom. count  
iff.

There exists symmetric and acyclic structure that dist. the structure by hom.  
count

- From this, restriction to symmetric structures is possible

## Conclusion

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- We presented classical CR and Scheidt's and Schweikardt's RCR algorithm
- We defined two possible ways to apply their algorithm to non-relational signatures
- We showed a logical characterisation for each of the approaches
- We disproved the characterisation by homomorphism counting
- We showed results for two restrictions of relational structures