Canonicalization of Data Structures

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Bled, February 2018
Introduction

Model
A mathematical object in some class $M$.

Example: a rational number, $\frac{3}{4}$
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An object of an abstract data type $R$ used to store the model.
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An object of an abstract data type $R$ used to store the model.
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Implementation
An object of a concrete type used to store the model.
Example: `std::pair<int, int>(3, 4)`
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A mathematical object in some class \( M \).

Example: a rational number, \( \frac{3}{4} \)

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An object of an abstract data type \( R \) used to store the model.

Example: a pair of integers, \((3, 4)\)

Implementation
An object of a concrete type used to store the model.

Example: `std::pair<int, int>(3, 4)`

What if a model has multiple representations?

Example
\( M = \mathbb{Q} \), the rational numbers
\( R = \mathbb{Z} \times \mathbb{Z} \), pairs of integers
But \( \frac{2}{5} = \frac{4}{10} \), so \((2, 5)\) should be considered “equal” to \((4, 10)\).

Notation: \((2, 5) \cong (4, 10)\) ("isomorphic to")
\((2, 5) \equiv (2, 5)\) ("representationally equal to")
**Canonicalization**

Given a representation \( G \in R \) find a new representation \( C(G) \), such that:

- It represents the same model: \( C(G) \cong G \)
- All canonicalized isomorphic representations are the same:
  \[
  \forall G' \in R, G' \cong G : \quad C(G') \cong r C(G)
  \]

How do we specify and implement canonicalization in practice?
Representations

Besides the \(\equiv_r\) operation we need:
- A class of operations, \(\mathcal{O}_P\), that do not change the model.
- A total order \(\prec_r\) among (isomorphic) representations.

Fraction Example:
\(\mathcal{O}_P\):
- Multiplying with an integer: \((2, 5) \cdot 2 = (2 \cdot 2, 5 \cdot 5) \equiv (2, 5)\)
- Dividing with a common factor: \(\frac{(4, 10)}{2} = \left(\frac{4}{2}, \frac{10}{2}\right) \equiv (4, 10)\)
- (and compositions of those operations)

\(\prec\):
- Prefer both positive over both negative: \((2, 5) \prec_r (-2, -5)\)
- Prefer (neg., pos.) over (pos., neg.): \((-2, 5) \prec_r (2, -5)\)
- Prefer smaller (absolute) numbers (lexicographically): \((2, 5) \prec_r (4, 10), (1, 2) \prec_\prec_r (2, 3)\)
Canonicalization

Given $G \in R$:

- Find $op \in \mathcal{O}_P$ that minimizes $op(G)$, wrt. $\prec$.
- Return $op(G)$ as the canonical form.

Fraction Example:

Given $(a, b)$,

- Find $f = GCD(|a|, |b|)$
- If $b < 0$: let $op = \text{DIV}(f) \circ \text{MUL}(-1)$
  - else: let $op = \text{DIV}(f)$
- Return $op((a, b))$

In Practice:

- Probably return $op$. The user can compute $op(G)$ if needed.
- $\prec$ may be implicitly defined by the canonicalization algorithm.
Example: Circular RNA (circRNA)

**Representation:** A sequence of symbols A, C, G, U.

**Example:** AGUGCAGUGGC

**Operations:** \( \text{ROTATE}(i) \), for \( i \in \mathbb{Z} \)

**Example:** \( \text{ROTATE}(2, \text{AGUGCAGUGGC}) = \text{UGCAGUGGCAG} \)

\( r \) and \( \triangleq \): component-wise and lexicographic comparison

**Canonicalization:** find the lexicographically smallest rotation
(can be done in linear time)
Example: Circular RNA (circRNA)

**Representation:** A sequence of symbols A, C, G, U.
Example: AGUGCAGUGC

**Operations:** Rotate \( i \), for \( i \in \mathbb{Z} \)
Example: Rotate(2, AGUGCAGUGC) = UGCAGUGCGAC

\( r \) and \( \leq \): component-wise and lexicographic comparison

**Canonicalization:** find the lexicographically smallest rotation
(can be done in linear time)

**Symmetry Discovery:** \( \text{op} \) is a symmetry if \( \text{op}(G) \leq G \)
Example: Rotate(5) is a symmetry of AGUGCAGUGC, because
Rotate(5, AGUGCAGUGC) = AGUGCAGUGC
\( \leq \) AGUGCAGUGC

Rotate(0) is a trivial symmetry
Example: Double Stranded RNA

Representation:
A pair of sequences of symbols A, C, G, U, of equal length.
Example: \begin{align*}
&\text{AGUGC} \\
&\text{UCACG}
\end{align*}

Operations: \text{REVERSE} \circ \text{SWAP}
Example: \begin{align*}
&\left( \text{REVERSE} \circ \text{SWAP} \right) \left( \begin{array}{c} AGUGC \\ UCACG \end{array} \right) = \begin{array}{c} GCACU \\ CGUGA \end{array}
\end{align*}

\text{r} = \text{and} \quad r^<: \text{component-wise and lexicographic comparison}
Example: \begin{align*}
&\begin{array}{c} AGUGC \\ UCACG \end{array} r^< \begin{array}{c} GCACU \\ CGUGA \end{array}
\end{align*}

Canonicalization: take the \text{r}^-\text{-smallest of the two possibilities}
Example: Double Stranded RNA, Only Binding Structure

Swapping all A with U and G with C preserves structure.

Representation:
A pair of sequences of symbols A, C, G, U, of equal length.

Operations: \( \text{REVERSE} \circ \text{SWAP} \) and \( \text{INVERT} (\equiv \text{SWAP}) \)

Example: \( \text{INVERT} \left( \begin{array}{c} AGUGC \\ UCACG \end{array} \right) = \left( \begin{array}{c} UCACG \\ AGUGC \end{array} \right) \)

\( \preceq \) and \( \prec \): component-wise and lexicographic comparison

Canonicalization: take the \( \prec \)-smallest of the four possibilities
Example: Anti-Parallel Strong Traces, Take 1

Model: A graph $G$ (representing a polygon), with a closed walk visiting all edges twice and $\langle$more constraints$\rangle$.

Representation: A sequence of vertices $t = (v_{i_1}, v_{i_2}, \ldots, v_{i_{2m}})$.

Operations: \textsc{Reverse}(t), \textsc{Rotate}(i, t), and \textsc{Permute}(\gamma, t) for any automorphism (i.e., symmetry) $\gamma$ of $G$.

$r \equiv$ and $r <$: component-wise and lexicographic comparison

Canonicalization: take the $r$-smallest (not trivial to do efficiently)

[Bašić et al., MATCH, 2017] [Hellmuth et al., ALENEX, 2018]
Example: Anti-Parallel Strong Strong Traces, Take 1

Model: A graph $G$ (representing a polygon), with a closed walk visiting all edges twice and \langle more constraints\rangle.

Representation: A sequence of vertices $t = (v_{i_1}, v_{i_2}, \ldots, v_{i_{2m}})$.

Operations: $\text{REVERSE}(t)$, $\text{ROTATE}(i, t)$, and $\text{PERMUTE}(\gamma, t)$ for any automorphism (i.e., symmetry) $\gamma$ of $G$.

$r = \text{and } <$: component-wise and lexicographic comparison

Canonicalization: take the $<-$smallest (not trivial to do efficiently)

But what about the graph?
What is a vertex?
What is the representation?

[Bašić et al., MATCH, 2017]
Example: Graphs, Part 1

Model: A graph $G = (V, E)$.

Representation: An adjacency list which implicitly assigns $1, 2, \ldots, n$ to $V$.

Operations: $\text{PERMUTE}(\gamma)$ for any permutation of $1, 2, \ldots, n$.

$r = r$ and $r <$: component-wise and lexicographic comparison

Canonicalization: ⟨more on this later⟩
Graph Representation and Graph Permutation

\[ G = (V, E) \quad V = \{1, 2, \ldots, n\} \]

Isomorphic graphs, different representations:

\[ G_1 \quad G \quad G_2 \]

Adjacency list representation (with sorted neighbour lists):

1: 4
2: 3, 4
3: 2, 4
4: 1, 2, 3

1: 2, 3, 4
2: 1
3: 1, 4
4: 1, 3

1: 4
2: 3, 4
3: 2, 4
4: 1, 2, 3
Graph Representation and Graph Permutation

\[ G = (V, E) \quad V = \{1, 2, \ldots, n\} \]

Isomorphic graphs, different representations:

\[ \pi_1 = (1\ 2\ 4)(3) \]

\[ \pi_2 = (1\ 2\ 3\ 4) \]

Adjacency list representation (with sorted neighbour lists):

\begin{align*}
1: & \quad 4 \\
2: & \quad 3, 4 \\
3: & \quad 2, 4 \\
4: & \quad 1, 2, 3 \\
\end{align*}

\begin{align*}
1: & \quad 2, 3, 4 \\
2: & \quad 1 \\
3: & \quad 1, 4 \\
4: & \quad 1, 3 \\
\end{align*}

\begin{align*}
1: & \quad 4 \\
2: & \quad 3, 4 \\
3: & \quad 2, 4 \\
4: & \quad 1, 2, 3 \\
\end{align*}
Example: Anti-Parallel Strong Traces, Take 2

Model: A graph $G$ (representing a polygon), with a closed walk visiting all edges twice and ⟨more constraints⟩.

Representation: An adjacency list, and a sequence of integers $t = (v_{i_1}, v_{i_2}, \ldots, v_{i_{2m}})$.

Operations:

- **REVERSE**$(t)$
- **ROTATE**$(i, t)$
- **PERMUTE**$(\gamma, t)$ for any automorphism $\gamma$ of $G$.
- **PERMUTE**$(\gamma, t, G)$ for any permutation $\gamma$ of $V$.

$\equiv$ and $\prec$: component-wise and lexicographic comparison

Canonicalization: take the $\prec$-smallest

[Bašić et al., MATCH, 2017]
Example: Anti-Parallel Strong Traces, Take 3

Model: A graph G (representing a polygon), with a closed walk visiting all edges twice and \langle \text{more constraints} \rangle.

Representation: An adjacency list, and a sequence of integers representing a gap vector $g = (a_1, a_2, \ldots a_{2m})$.

![Diagram of a square pyramid with vertex strong trace $t = (0, 2, 1, 4, 2, 0, 3, 4, 1, 3, 0, 4, 3, 1, 2, 4)$ and gap vector $g = (5, 3, 6, 4, 10, 5, 3, 4, 5, 3, 6, 4, 10, 5, 3, 4)$]

[Hellmuth et al., ALENEX, 2018]
**Example: Anti-Parallel Strong Traces, Take 3**

**Model:** A graph $G$ (representing a polygon), with a closed walk visiting all edges twice and ⟨more constraints⟩.

**Representation:** An adjacency list, and a sequence of integers representing a *gap vector* $g = (a_1, a_2, \ldots a_{2m})$.

**Operations:**
- $\text{ROTATE}(i, g)$
- $\text{MAKE GAP} \circ \text{REVERSE} \circ \text{MAKE TRACE}$

$r \equiv$ and $r <$: component-wise and lexicographic comparison

**Canonicalization:** find the $r$-smallest rotation of $g$ and its reverse.

[Hellmuth et al., ALENEX, 2018]
Example: Graphs, Continued

Model: A graph \( G = (V, E) \).

Representation: An adjacency list which implicitly assigns \( 1, 2, \ldots, n \) to \( V \).

Operations: \( \text{PERMUTE}(\gamma) \) for any permutation of \( 1, 2, \ldots, n \).

\( \preceq \) and \( \prec \): component-wise and lexicographic comparison

Computational Complexity: \( \exp \left( O \left( \sqrt{n \log n} \right) \right) \)

Brute-Force Algorithm:

1. Construct \( G^\gamma \) for all permutations \( \gamma \in S_n \).
2. Select the “best” one (for example the \( \preceq \)-smallest).


Existing Tools for Canonicalization in Practice

Published Tools: nauty, Traces, Bliss (and Saucy and Conauto)

- All based on the idea of individualization-refinement.
- Different sets of heuristics and variations.
- Many more algorithm variations are possible.
- Which is the best? for a specific class of graphs?
- What if the graph has vertex and edge labels?
- What if those labels are “complicated”? (e.g., stereo-info)

Existing Tools for Canonicalization in Practice

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- What if those labels are “complicated”? (e.g., stereo-info)

GraphCanon: [Andersen and Merkle, ALENEX, 2018]

- A generic C++ library for canonization algorithms.
- Algorithm variations implementable as individual plugins.
- Allows direct comparison of algorithm variations.
- Lower barrier of entry for implementing new ideas.
- Generality wrt. vertex/edge attributes.

Individualization-Refinement Paradigm

Initially: all vertices are unordered (same colour).
Individualization-Refinement Paradigm

Refine the ordering by propagation of “cheap” local information. **Example**: sort and partition by degree (1D Weisfeiler-Leman).

![Graph example]

1 2 3 4 5 6 7 8 9 10

![Partitioned graph example]

[1 2 3 4 5 6 7 8 9 10]

[1 2 | 3 4 5 6 7 8 9 10]
Individualization-Refinement Paradigm

Refine the ordering by propagation of “cheap” local information. **Example:** sort and partition by degree (1D Weisfeiler-Leman).

![Diagram](image-url)
Individualization-Refinement Paradigm

Let this be the root of a search tree, and select a colour. For each vertex of that colour;
create a child with this vertex given a unique new colour.
Individualization-Refinement Paradigm

\[ \pi(1) = [1 | 2 | 7 | 8 | 9 | 10 | 5 | 6 | 3 | 4] \]

\[ \pi(2) = [2 | 1 | 7 | 8 | 9 | 10 | 3 | 4 | 5 | 6] \]

\[ \pi(1,7) = [1 | 2 | 7 | 10 | 8 | 9 | 6 | 5 | 4 | 3] \]

\[ \pi(2,7) = [2 | 1 | 7 | 10 | 8 | 9 | 4 | 3 | 6 | 5] \]

\[ \pi(1,8) = [1 | 2 | 8 | 9 | 7 | 10 | 5 | 6 | 3 | 4] \]

\[ \pi(1,9) = [1 | 2 | 9 | 8 | 10 | 7 | 6 | 5 | 3 | 4] \]
Algorithm Variation

Categories

- Tree traversal
- Target cell selection
- Refinement
- Pruning with automorphisms
- Detection of implicit automorphisms
- Node invariants

GraphCanon: A common extension infrastructure.

Each variation implemented as a visitor:

- A set of callback methods for events of interest.
- Additional data structures instantiated
  - per search tree
  - per tree node
Benchmarks

44 graph collections, with 4,715 graphs in total.
Time limit: 1000 s
Memory limit: 8 GB
Repetitions: 5

Algorithm configurations: \{BFSExp, DFS\} × \{F, FL, FLM\}

Compute nodes with two Intel E5-2680v3 CPUs (24 cores)
Compute node hours: approx. 12,000

BFSExp with FLM is often best.

CFI-Rigid: [Neuen and Schweitzer, ESA, 2017]
nauty, Traces: [http://pallini.di.uniroma1.it/Graphs.html]
Conauto: [https://sites.google.com/site/giconauto/home/benchmarks]
Saucy: [http://vlsicad.eecs.umich.edu/BK/SAUCY/]
Tree Traversal and Target Cell Selector

Similar characteristics observed for other Miyazaki graphs.
Tree Traversal and Target Cell Selector

usr, Union of Strongly Regular Graphs

- nauty (d)
- nauty (s)
- Traces
- Bliss
- BFSExp-F
- BFSExp-FL
- BFSExp-FLM
- DFS-F
- DFS-FL
- DFS-FLM
CFI-Rigid

- 6 collections
- Designed to be the hard benchmarks.
- Expected to have very little symmetry.

Algorithm configurations:

\[
\{\text{BFSExp, DFS}\} \times \{F, FL, FLM\} \times 2^{\{PL, Q, T\}}
\]

<table>
<thead>
<tr>
<th>Col. Group</th>
<th>Reduction</th>
<th>Best Algorithm</th>
<th>Invariants Matter</th>
<th>FLM Sep.</th>
<th>Max. Solved</th>
<th>Solved n</th>
</tr>
</thead>
<tbody>
<tr>
<td>d3</td>
<td>$D_3$</td>
<td>—</td>
<td>BFSExp-FLM</td>
<td>yes (any)</td>
<td>yes</td>
<td>3,600</td>
</tr>
<tr>
<td>z3</td>
<td>$\mathbb{Z}_3$</td>
<td>—</td>
<td>BFSExp-FLM</td>
<td>yes (any)</td>
<td>yes</td>
<td>3,780</td>
</tr>
<tr>
<td>z2</td>
<td>$\mathbb{Z}_2$</td>
<td>—</td>
<td>Bliss, nauty (s)</td>
<td>yes (any)</td>
<td>no</td>
<td>2,992</td>
</tr>
<tr>
<td>r2</td>
<td>$\mathbb{Z}_2 \times R^*$</td>
<td>Bliss, nauty (s)</td>
<td>no</td>
<td>no</td>
<td>1,584</td>
<td></td>
</tr>
<tr>
<td>s2</td>
<td>$\mathbb{Z}_2 \times B^*$</td>
<td>FLM, Bliss, nauty (s)</td>
<td>yes (PL or Q)</td>
<td>no</td>
<td>2,496</td>
<td></td>
</tr>
<tr>
<td>t2</td>
<td>$\mathbb{Z}_2 \times R^* \circ B^*$</td>
<td>FLM, Bliss, nauty (s)</td>
<td>yes (PL or Q)</td>
<td>yes</td>
<td>1,056</td>
<td></td>
</tr>
</tbody>
</table>
CFI-Rigid

The graph shows the time (in seconds) on the y-axis against the number of nodes (n) on the x-axis. The graph includes data points for different algorithms:

- nauty (d)
- nauty (s)
- Traces
- Bliss
- BFSExp-F
- BFSExp-FL
- BFSExp-FLM
- DFS-F
- DFS-FL
- DFS-FLM

Key markers indicate OOM and OOT (Out of Memory and Out of Time) limits.
Summary

- Canonicalization is a general principle.
- The concepts can be applied to any data structure.
- Brute-force: make it a graph.

GraphCanon:

- Generic algorithm framework.
- (Relatively) easy to develop new variations.
- Allows direct comparison of algorithmic ideas.
- Competitive with established tools.
- https://github.com/jakobandersen/graph_canon
- Very easy to extract data for visualization:
  https://jakobandersen.github.io/graph_canon_vis/

MØD v0.7 (to be released soon™):

- Integrates GraphCanon.
- Finally, true canonical SMILES strings!
- The automorphism group of molecules is now available.
  (important for atom tracing)
Algorithm Variation

Tree Traversal:
- **nauty, Bliss**: depth-first (DFS)
- **Traces**: breadth-first with experimental paths (BFSExp)
- **GraphCanon**:
  - Arbitrary traversals are possible.
  - Garbage collected search tree via reference counting.
  - Extensions must keep owning references to tree nodes.
  - Implemented: DFS, BFSExp, and a new hybrid (BFSExpM).

Target Cell Selector:
- Many have been developed.
- Currently implemented:
  - first (F)
  - first largest (FL)
  - first largest with maximum number of non-uniformly joined neighbour cells (FLM)
Algorithm Variation

Node Invariants:

- Totally ordered isomorphism-invariant information.
- Invariants can be implemented independently.
- A special visitor coordinates invariants.
- Implemented:
  - cell splitting positions (T), from Traces
  - quotient graph values (Q), from nauty, Traces, Bliss (but not hashed)
  - partial leaf (PL), from Bliss (but not hashed)
  
    Construct parts of the permuted graph earlier in the tree.

Refinement functions implemented:

- 1D Weisfeiler-Leman, generalized to exploit edge attributes.
- A function to handle degree-1 vertices.
Algorithm Variation

Detection of implicit automorphisms:

▶ Sometimes we can detect/guess automorphisms at internal tree nodes.
▶ **nauty**: several special cases of ordered partitions.
▶ **Saucy**: heuristics for guessing sparse automorphisms.
▶ **Traces**: reportedly a generalization of the Saucy heuristics.
▶ **Implemented**:
  ▶ Partitions where all cells have size 1 or 2.
  ▶ The degree-1 vertex refinement function.

Pruning with automorphisms:
Calculation of orbits in stabilizers of the found automorphisms.

Stabilizer calculation:

▶ **nauty** (early versions) and **Bliss**: conservative (implemented)
▶ **Traces** and **nauty** (recent versions): randomized Schreier-Sims

The implemented visitor for automorphism pruning is generic with respect to stabilizer implementation.