Canonicalization of Data Structures

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Introduction

Model

A mathematical object in some class M.

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

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

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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”)

$(2, 5) \stackrel{r}{=} (2, 5)$ (“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:
  $\forall G' \in R, G' \cong G : \quad C(G') \stackrel{r}{=} C(G)$

How do we specify and implement canonicalization in practice?

Representations

Besides the $\stackrel{r}{=}$ operation we need:

- A class of operations, $\textsc{Op}$, that do not change the model.
- A total order $\stackrel{r}{<}$ among (isomorphic) representations.

Fraction Example:

$\textsc{Op}$:

- Multiplying with an integer: $(2,5)\cdot 2 = (2\cdot 2, 5\cdot 5) \cong (2,5)$
- Dividing with a common factor: $\frac{(4,10)}{2} = \left(\frac{4}{2}, \frac{10}{2}\right) \cong (4,10)$
- (and compositions of those operations)

$\stackrel{r}{<}$:

- Prefer both positive over both negative: $(2,5) \stackrel{r}{<} (-2,-5)$
- Prefer (neg., pos.) over (pos., neg.): $(-2,5) \stackrel{r}{<} (2,-5)$
- Prefer smaller (absolute) numbers (lexicographically): $(2,5) \stackrel{r}{<} (4,10), \quad (1,2) \stackrel{r}{<} (2,3)$

Canonicalization

Given $G \in R$:

- Find $op \in \textsc{Op}$ that minimizes $op(G)$, wrt. $\overset{r}{<}$
- Return $op(G)$ as the canonical form.

Fraction Example:

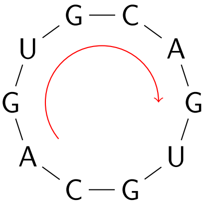
Given (a, b),

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

In Practice:

- Probably return op. The user can compute $op(G)$ if needed.
- $\overset{r}{<}$ may be implicitly defined by the canonicalization algorithm.

Example: Circular RNA (circRNA)



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

Operations: $\textsc{Rotate}(i)$, for $i \in \mathbb{Z}$
  Example: $\textsc{Rotate}(2, \text{AGUGCAGUGC}) = \text{UGCAGUGCAG}$

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

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

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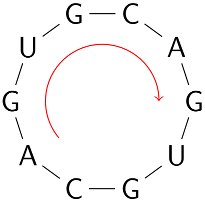

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Symmetry Discovery: op is a symmetry if $op(G) \overset{r}{=} G$
  Example: $\textsc{Rotate}(5)$ is a symmetry of AGUGCAGUGC, because

$$\begin{aligned} \textsc{Rotate}(5, \text{AGUGCAGUGC}) &= \text{AGUGCAGUGC} \\ &\overset{r}{=} \text{AGUGCAGUGC} \end{aligned}$$

$\textsc{Rotate}(0)$ is a trivial symmetry

Example: Double Stranded RNA

Representation:

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

Example: $\begin{smallmatrix}\mathsf{AGUGC}\\\mathsf{UCACG}\end{smallmatrix}$

Operations: $\textsc{Reverse} \circ \textsc{Swap}$

Example: $(\textsc{Reverse} \circ \textsc{Swap}) \binom{\mathsf{AGUGC}}{\mathsf{UCACG}} = \begin{smallmatrix}\mathsf{GCACU}\\\mathsf{CGUGA}\end{smallmatrix}$

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

Example: $\begin{smallmatrix}\mathsf{AGUGC}\\\mathsf{UCACG}\end{smallmatrix} \stackrel{r}{<} \begin{smallmatrix}\mathsf{GCACU}\\\mathsf{CGUGA}\end{smallmatrix}$

Canonicalization: take the $\stackrel{r}{<}$-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: $\textsc{Reverse} \circ \textsc{Swap}$ and $\textsc{Invert}$ $(= \textsc{Swap})$
Example: $\textsc{Invert}\begin{pmatrix}\mathsf{AGUGC}\\ \mathsf{UCACG}\end{pmatrix} = \begin{pmatrix}\mathsf{UCACG}\\ \mathsf{AGUGC}\end{pmatrix}$

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

Canonicalization: take the $\stackrel{r}{<}$-smallest of the four possibilities

Example: Anti-Parallel Strong Traces, Take 1

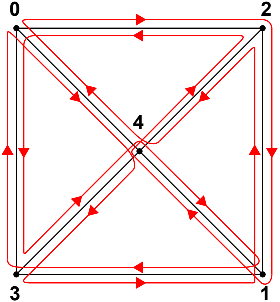
Model: A graph G (representing a polygon), with a closed walk visiting all edges twice and $\langle$more constraints$\rangle$.

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) γ of G.

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

Canonicalization: take the $\overset{r}{<}$-smallest (not trivial to do efficiently)



[Hellmuth et al., ALENEX, 2018]

[Bašić et al., MATCH, 2017]

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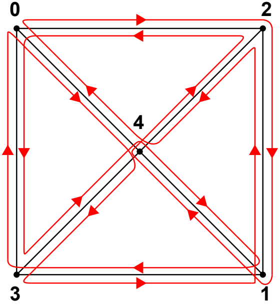


[Hellmuth et al., ALENEX, 2018]

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: $\textsc{Permute}(\gamma)$ for any permutation of $1, 2, \ldots, n$.

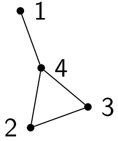
$\overset{r}{=}$ and $\overset{r}{<}$: component-wise and lexicographic comparison

Canonicalization: $\langle$more on this later$\rangle$

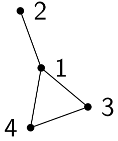
Graph Representation and Graph Permutation

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

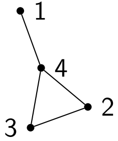
Isomorphic graphs, different representations:



G_1



G



G_2

Adjacency list representation (with sorted neighbour lists):

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

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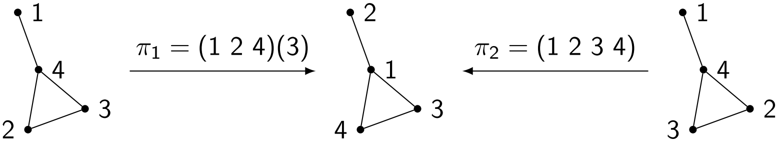
$G = (V, E) \quad V = \{1, 2, \ldots, n\}$

Isomorphic graphs, different representations:



G_1 $\qquad G_1^{\pi_1} \stackrel{r}{=} G \stackrel{r}{=} G_2^{\pi_2}$ $\qquad G_2$

Adjacency list representation (with sorted neighbour lists):

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

Example: Anti-Parallel Strong Traces, Take 2

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

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

Operations:

- $\textsc{Reverse}(t)$
- $\textsc{Rotate}(i, t)$
- $\textsc{Permute}(\gamma, t)$ for any automorphism γ of G.
- $\textsc{Permute}(\gamma, t, G)$ for any permutation γ of V.

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

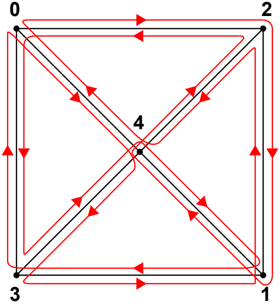
Canonicalization: take the $\overset{r}{<}$-smallest

[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 $\langle$more constraints$\rangle$.

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



$$t = (0, 2, 1, 4, 2, 0, 3, 4, 1, 3, 0, 4, 3, 1, 2, 4)$$
$$g = (5, 3, 6, 4, 10, 5, 3, 4, 5, 3, 6, 4, 10, 5, 3, 4)$$

[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 $\langle$more constraints$\rangle$.

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

Operations:

- $\textsc{Rotate}(i, g)$
- $\textsc{MakeGap} \circ \textsc{Reverse} \circ \textsc{MakeTrace}$

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

Canonicalization: find the $\overset{r}{<}$-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 $1, 2, \dots, n$ to V.

Operations: $\textsc{Permute}(\gamma)$ for any permutation of $1, 2, \dots, n$.

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

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

Brute-Force Algorithm:

1. Construct G^γ for all permutations $\gamma \in S_n$.
2. Select the "best" one (for example the $\stackrel{r}{<}$-smallest).

[Babai and Luks, STOC, 1983]

[Babai, Handbook of Combinatorics, 1996]

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)

[McKay, Congressus Numerantium, 1981] [McKay and Piperno, J. Symb. Comp., 2014] [Junttila and Kaski, ALENEX, 2007] [Darga et al., DAC, 2008] [López-Presa and Fernández Anta, SEA, 2009]

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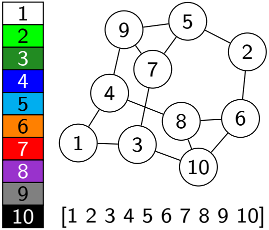
GraphCanon: [Andersen and Merkle, ALENEX, 2018]

- 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.

[McKay, Congressus Numerantium, 1981] [McKay and Piperno, J. Symb. Comp., 2014] [Junttila and Kaski, ALENEX, 2007] [Darga et al., DAC, 2008] [López-Presa and Fernández Anta, SEA, 2009]

Individualization-Refinement Paradigm

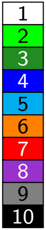
Initially: all vertices are unordered (same colour).

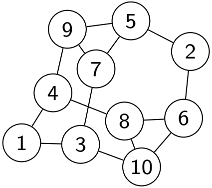


Individualization-Refinement Paradigm

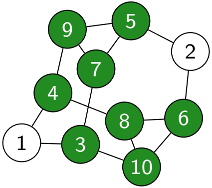
Refine the ordering by propagation of “cheap” local information.

Example: sort and partition by degree (1D Weisfeiler-Leman).





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



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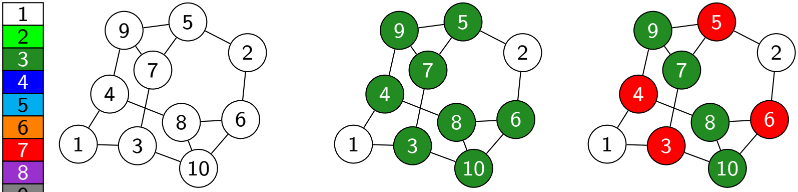


[1 2 3 4 5 6 7 8 9 10]

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

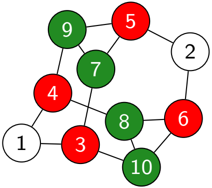
[1 2 | 7 8 9 10 | 3 4 5 6]

Individualization-Refinement Paradigm

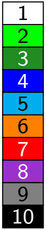
Let this be the root of a search tree, and select a colour.

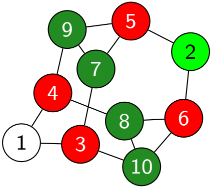
For each vertex of that colour;

create a child with this vertex given a unique new colour.

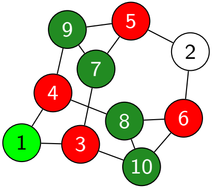


[1 2 | 7 8 9 10 | 3 4 5 6]



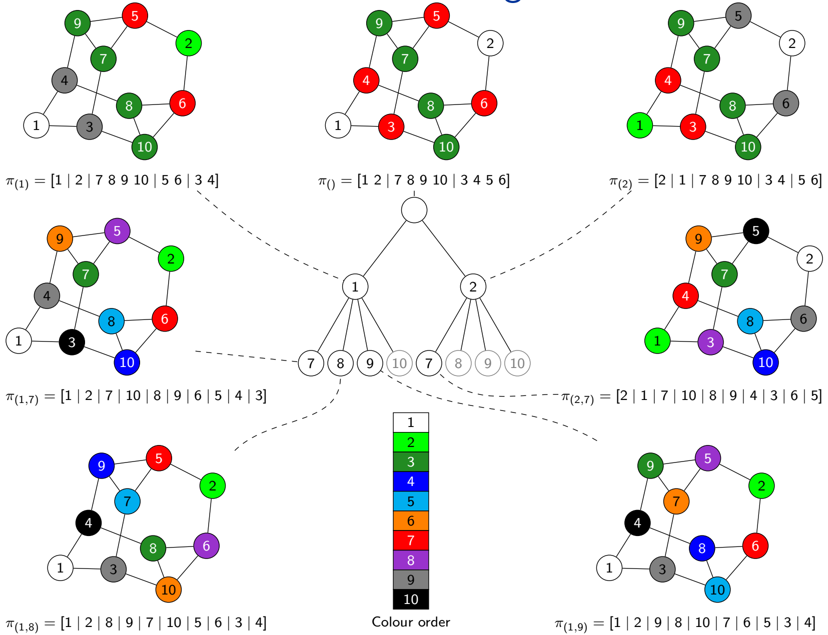


[1 | 2 | 7 8 9 10 | 3 4 5 6]



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

Individualization-Refinement Paradigm



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

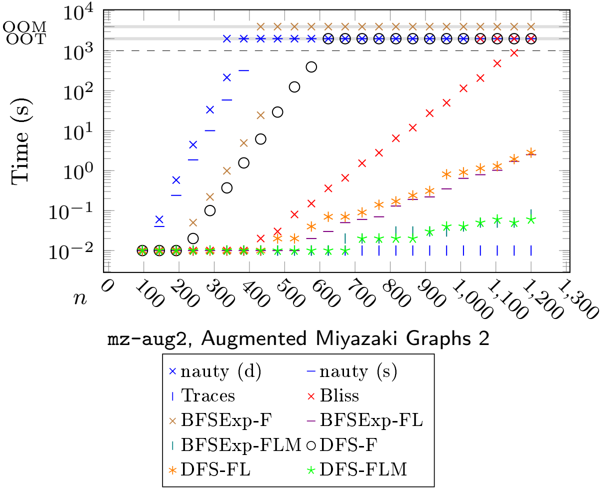
Algorithm configurations: $\{\mathrm{BFSExp}, \mathrm{DFS}\} \times \{\mathrm{F}, \mathrm{FL}, \mathrm{FLM}\}$

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]
Bliss: [http://www.tcs.hut.fi/Software/bliss/benchmarks/index.shtml]
Conauto: [https://sites.google.com/site/giconauto/home/benchmarks]
Saucy: [http://vlsicad.eecs.umich.edu/BK/SAUCY/]

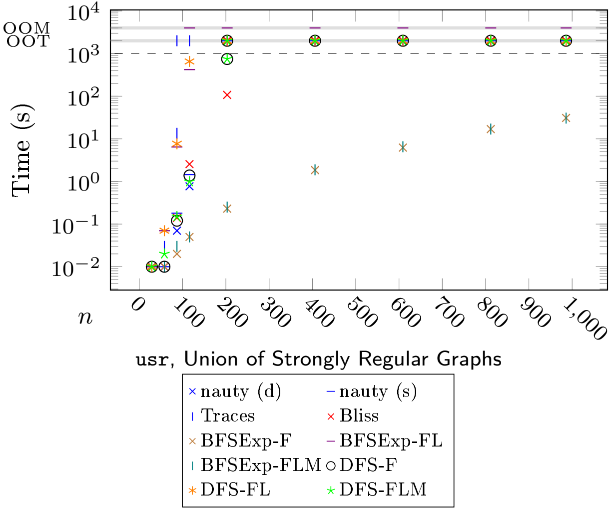
Tree Traversal and Target Cell Selector



`mz-aug2`, Augmented Miyazaki Graphs 2

Similar characteristics observed for other Miyazaki graphs.

Tree Traversal and Target Cell Selector



usr, Union of Strongly Regular Graphs

CFI-Rigid

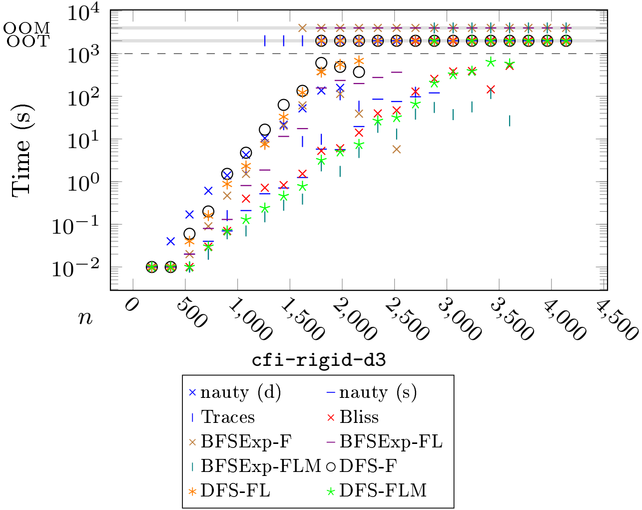
- 6 collections
- Designed to be the hard benchmarks.
- Expected to have very little symmetry.

Algorithm configurations:

$$\{\mathrm{BFSExp}, \mathrm{DFS}\} \times \{\mathrm{F}, \mathrm{FL}, \mathrm{FLM}\} \times 2^{\{\mathrm{PL}, \mathrm{Q}, \mathrm{T}\}}$$

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

CFI-Rigid



10^4
OOM
OOT
10^3
10^2
10^1
10^0
10^{-1}
10^{-2}
Time (s)
n
0
500
1,000
1,500
2,000
2,500
3,000
3,500
4,000
4,500
cfi-rigid-d3
nauty (d)
nauty (s)
Traces
Bliss
BFSExp-F
BFSExp-FL
BFSExp-FLM
DFS-F
DFS-FL
DFS-FLM

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)

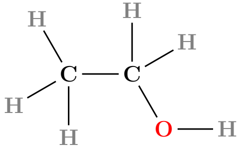
Algorithm Variation

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.