On the Weisfeiler-Leman Dimension of Fractional Packing

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Outline

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1-WL = Color Refinement Procedure

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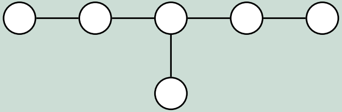

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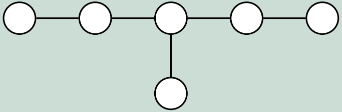

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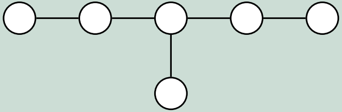

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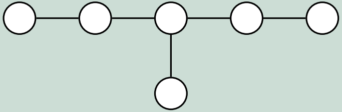

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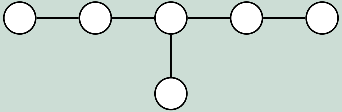

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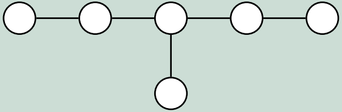

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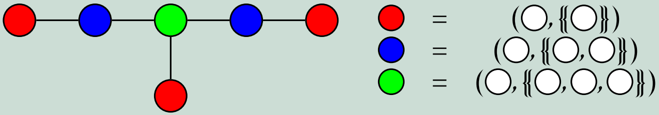

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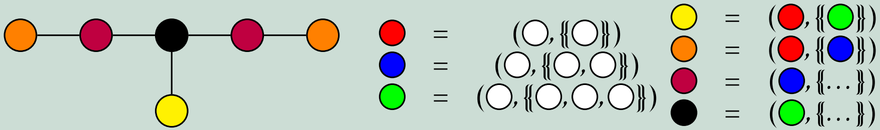

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Input: n-vertex (colored) graph $G = (V, E)$, $\bar{x} \in V^k$

- We let $\mathrm{WL}_k^0(G, \bar{x})$ encode the colored *isomorphism type* of $\bar{x}$ in G. For $k = 2$ this means *identity*, *edge* or *non-edge* plus edge/vertex color.
- $\mathrm{WL}_k^r(G, \bar{x}) = (\mathrm{WL}_k^{r-1}(G, \bar{x}), \{\!\{(\mathrm{WL}_k^{r-1}(G, \bar{x}_1^u), \dots, \mathrm{WL}_k^{r-1}(G, \bar{x}_k^u)) : u \in V(G)\}\!\})$, where $\bar{x}_i^u$ is the tuple $(x_1, \dots, x_{i-1}, u, x_{i+1}, \dots, x_k)$. This means we put each vertex $u \in V$ in each possible position of the tuple and query the current color.
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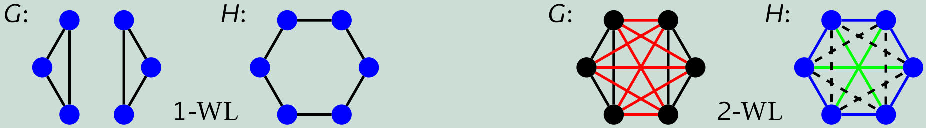
- For $k = 2$ this means counting colored triangle extensions for ordered pairs.

Example (1-WL vs. 2-WL)



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- There is an algorithm [Cardon, Crochemore 1982] that generalizes both this second approach and Hopcroft's DFA minimization.
- Some real live isomorphism algorithms (e.g. nauty and Traces [McKay, Piperno 2014]) alternate refinement with recoloring single vertices and backtracking to obtain a canonical vertex order on a single input graph.

Usage in practice II

Graph kernels

A kernel function is used for, e.g., support vector machines to measure the similarity of objects. For graphs the Weisfeiler-Leman algorithm can be used to define a kernel roughly like this ("Weisfeiler-Lehman Subtree Kernel" [Shervashidze et al. 2011]):

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1. Run some number h of rounds on two graphs $G = (V, E), G'(V', E')$ in parallel.
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Graph neural networks

More involved methods combining k-WL and neural networks exist, see, e.g., [Morris et al. 2019]

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- We are specifically interested in parameter with WL dimension 1 or 2 as the running times of 1-WL and 2-WL are still acceptable for many practical purposes.

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Example (expressed in our terminology)

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A matching can be seen as a function $w\colon E \to \{0,1\}$ such that for each vertex u we have $\sum_{e \in E, u \in e} w(e) \leq 1$. Then the matching number ν is the maximal value $\sum_{e \in E} w(e)$ over all matchings.

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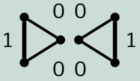
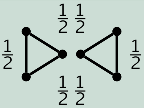
We can express ν as a solution of an integer linear programs and ν_f as the solution of its fractional relaxations. So by the fractional parameter π_f we will mean the solution of the fractional relation of the usual integer linear program for π.

Example

$\nu(2K_3) = 2$





$\nu_f(2K_3) = 6 \cdot \frac{1}{2} = 3$

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Why should fractional parameters have low WL dimension?

$G \equiv_{1\text{-WL}} H$ if and only if G and H are *fractionally isomorphic* [Scheinerman, Ullman 1997], i.e., there is a doubly stochastic matrix X such that $AX = XB$, where A and B are the adjacency matrices of G and H (X respects colors for colored graphs).
That is, 1-WL can be seen as a fractional relaxation of isomorphism.

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Definition

- The set packing problem (Set Packing) is to maximize the number of pairwise disjoint sets in a given family of sets $\mathcal{S} = \{S_1, \ldots, S_n\}$, where each $S_j \subset \{1, \ldots, m\}$. As $\mathcal{S}$ can be seen as a hypergraph, we also use $\nu(S)$ for the set packing number.

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- Its fractional analogue $\nu_f(\mathcal{S})$ is the optimal value of the following LP:

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\begin{aligned}
\max \sum_{i=1}^{n} x_i & \quad \text{under} \\
x_i & \geq 0 \text{ for every } i \leq n, \\
\sum_{i : S_i \ni j} x_i & \leq 1 \text{ for every } j \leq m.
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$$\begin{aligned} \max \sum_{i=1}^{n} x_i \quad & \text{under} \\ x_i \geq\ & 0 \text{ for every } i \leq n, \\ \sum_{i\,:\,S_i \ni j} x_i \leq\ & 1 \text{ for every } j \leq m. \end{aligned}$$

  Here each x_i expresses the weight of set S_i.
- Let $Inc(\mathcal{S}) = (V, E)$ denote the colored incidence graph of $\mathcal{S}$, i.e., $V = \{r_j : 1 \leq j \leq m\} \cup \{b_i : 1 \leq i \leq n\}$ and $E = \{r_j, b_i\} : j \in S_i\}$.

The (fractional) set packing problem II

Theorem (Theorem A)

Let $\mathcal{S}$ and $\mathcal{T}$ be two families each consisting of n subsets of the set $\{1, \ldots, m\}$. If $Inc(\mathcal{S}) \equiv_{\text{1-WL}} Inc(\mathcal{T})$, then $\nu_f(\mathcal{S}) = \nu_f(\mathcal{T})$.

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- If x is an optimal solution for $LP(\mathcal{T})$ then so is $x' = Zx$ for $LP(\mathcal{S})$ (and vice versa):

$$Mx' = \underbrace{MZ}_{YN} x = Y \underbrace{Nx}_{\leq \mathbb{1}} \leq Y\mathbb{1} = \mathbb{1} \quad \text{and} \quad \mathbb{1}^t x' = \underbrace{\mathbb{1}^t Z}_{\mathbb{1}^t} x = \mathbb{1}^t x.$$

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Example (Fractional matching number)

Let $G = (V, E)$ be a graph, then $\mathcal{S}_G$ is simply E. We show that $G \equiv_{\text{1-WL}} H$ implies $Inc(\mathcal{S}_G) \equiv_{\text{1-WL}} Inc(\mathcal{S}_H)$ and hence the WL dimension of ν_f is 1.

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Example (Fractional F-packing number)

The F-packing number $\pi^F(G)$ counts the maximal number of vertex disjoint subgraphs F in G (a matching is a K_2-packing). Here $\mathcal{S}_G$ is the family of all vertex sets of copies of F in G. Then $\pi^F(G) = \nu(\mathcal{S}_G)$ and we define $\pi^F_f(G) = \nu_f(\mathcal{S}_G)$.

Outline

Upper bound of the WL dimension of F-packing

Theorem

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Definition

A graph F has homomorphism-hereditary treewidth $htw(F) = k$ if the maximal treewidth over all its homomorphic images is k.

This means the maximal treewidth obtainable by merging non-adjacent vertices.

Example

Graphs F with $htw(F) \leq 2$ are, for instance, paths and cycles with up to 6 vertices and the 5-matching.

Upper bound of the WL dimension of F-packing

Theorem

If $htw(F) \leq k$, then π_f^F is k-WL-invariant.

Proof sketch.

- Given two graphs $G \equiv_{k\text{-WL}} H$, we can assume $V(G) = V(H)$ and that vertices x are colored with $c(x) = \mathrm{WL}_k(G, \underbrace{x, \dots, x}_{k \text{ times}}) = \mathrm{WL}_k(H, \underbrace{x, \dots, x}_{k \text{ times}})$.
- For each coloring of F, the color $c(x)$ "knows" in how many colored copies of F in G (or H) the vertex x appears (using [Dvořák 2010, Lemma 4] + [Lovász 2012, Section 5.2.3], see [F., Köbler, Verbitsky 2020] for details).
- We extend the coloring c of $V(G)$ to a coloring c^F of all the vertices of $Inc(\mathcal{S}_G)$, i.e., to the vertex sets $V(F')$ of copies F' of F: $c^F(V(F')) = \{\!\{c(x) : x \in V(F')\}\!\}$.
  c^F still corresponds to an equitable partition of $Inc(\mathcal{S}_G)$.
- The same can be done consistently for $H/Inc(\mathcal{S}_H)$ and thus by theorem Theorem A we have $\pi_f^F(G) = \pi_f^F(H)$. □

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- Let k be the WL dimension of a fractional parameter π_f. We define the integrality gap $IG^\pi = \sup_G \max(\frac{\pi_f(G)}{\pi(G)}, \frac{\pi(G)}{\pi_f(G)})$ (sup over all Graphs), the invariance ratio $IR^\pi = \sup_{G,H} \frac{\pi(G)}{\pi(H)}$ (sup over all $G \equiv_{k\text{-WL}} H, \pi(H) \neq 0$) and the invariance difference $ID^\pi(n) = \sup|\pi(G) - \pi(H)|$. (sup over all n-vertex $G \equiv_{k\text{-WL}} H$). Clearly, $IR^\pi \leq IG^\pi$.

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- For edge disjoint triangle packing, we get: $IG^{\rho^{K_3}} = IR^{\rho^{K_3}} = 2$ and $ID^{\rho^{K_3}}(n) = \Omega(n^{1.25})$.
- For the domination number, there are infinitely many n such that $IG^\gamma(n) \geq IR^\gamma(n) \geq (\frac{1}{4} - o(1))\log_2 n$.
  From [Lovász 1975] we already know: $IG^\gamma(n) \leq 1 + \ln n$.

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- Fractional parameters that are not instances of set packing or hitting set

Thank You!

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