On Counting Subgraphs and the Weisfeiler-Lehman Algorithm

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NCW 2018, Berlin

Outline

1. Properties, Retainment and the Weisfeiler-Lehman algorithm
2. Counting subgraphs
3. Retaining fractional graph parameters

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Properties and retainment

Definition

- Let $f : D \to A$ and $f : D \to B$ some functions on a common domain D. We say f *retains* g, if for every $x, y \in D$: $f(x) = f(y) \Rightarrow g(x) = g(y)$.

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Example

For possible domains think of

- $\mathcal{G}$: all graphs G with, say, $\exists n \in \mathbb{N} : V(G) = \{1, \ldots, n\}$.
- $\mathcal{G}_k$: all pairs (G, X) with $X \in V(G)^k, G \in \mathcal{G}$

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Retainments:

- Provided we assume that the $|V(G)|$ is always included in the parameters (true for Weisfeiler-Lehman), vc (smallest vertex cover) and is (largest independent set) are functions on $\mathcal{G}$ and retain each other, as $\mathrm{vc}(G) + \mathrm{is}(G) = |V(G)|$.
- Let $\mathrm{br}(G, u, v)$ be 1 if and only if $\{u, v\}$ is a bridge in G, else 0. Let $\mathrm{pl}(G, u, v) = \{(i, j) :$ there are i paths of length j from u to $v\}$. Then *pl* retains *br*.

k-dim. Weisfeiler-Lehman algorithm (k-WL)

Input: (possibly colored) graph G:

- For every $X = \{x_1 \dots, x_k\} \in V(G)^k$, define $C_G^0(X)$ as the ordered isomorphism type of the subgraph induced by X.
- If $i \geq 0$ and $k = 1$ (and thus X is some $u \in V(G)$), define:
  $C^{i+1}(u) = \left(C^i(u), \left\{\!\!\left\{ C^i(a) : a \in N(u) \right\}\!\!\right\}\right)$,
- else $C^{i+1}(X) = \left(C^i(X), \left\{\!\!\left\{ C'^i(X, v) : v \in V(G) \right\}\!\!\right\}\right)$ where
  $C'^i(X, v) = \left(C^i(v, x_2, \dots), \dots, C^i(x_1, \dots, x_{k-1}, v)\right)$
- In both cases $C^\infty(X) = \left\{(i, C^i(X)) : i \geq 0\right\}$.
- Practical application requires renaming the colors (to avoid expobential size) and then parallel application in a pair of graphs. We will stick with $C^\infty(X)$ for this talk.

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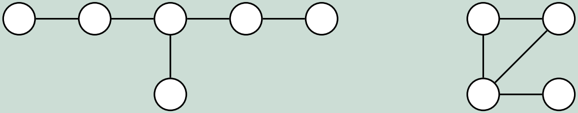

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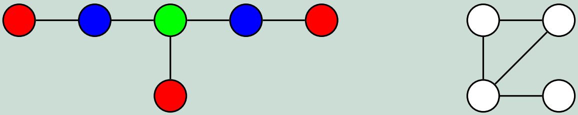

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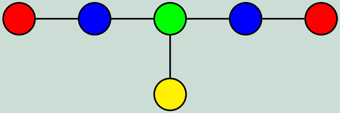

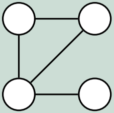

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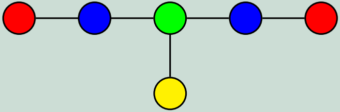

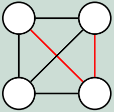

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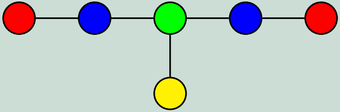

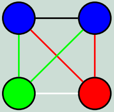

k-dim. Weisfeiler-Lehman algorithm (k-WL)

Natural properties based on k-WL

- $f_{k\text{-WL-local}}(G, X) = C^\infty(X)$ on $\mathcal{G}_k$
- $f_{k\text{-WL}}(G) = \{\!\{ C^\infty(X) : X \in V(G)^k \}\!\}$ on $\mathcal{G}$
- We say $G \equiv_{k\text{-WL}} H$ if $f_{k\text{-WL}}(G) = f_{k\text{-WL}}(H)$

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Example

$f_{2\text{-WL-local}}(G, u, v)$ retains the walks of any length between u and v,
$f_{2\text{-WL}}$ retains the spectrum.

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Question

Which other properties does k-WL retain?

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Subgraph counts

Definition

- Let $\mathrm{sub}_F(G)$ be the number of subgraphs of G isomorphic to the pattern graph F, and $\mathrm{rec}_F(G) = 1$ if $\mathrm{sub}_F(G) \geq 0$, else 0.

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Results from [Fürer 17]

- $K_4 \notin \mathcal{C}(2)$
- $C_s \in \mathcal{C}(2)$ for $s \leq 6$
- $C_s \notin \mathcal{C}(2)$ for $8 \geq s \leq 16$

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Our Results regarding subgraphs

- Complete characterization of $\mathcal{C}(1)$ and $\mathcal{R}(1)$
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Complete characterization of $\mathcal{C}(1)$ and $\mathcal{R}(1)$

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$\mathcal{C}(1) = \{ K_{1,s} : s \geq 1 \} \cup \{2K_2\}$

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Proof.

The positive instances can be derived from the degree sequence:
$\mathrm{sub}_{K_{1,s}}(G) = \sum_{v \in V(G)} \binom{\deg v}{s}$ and $\mathrm{sub}_{2K_2}(G) = \binom{e(G)}{2} - \mathrm{sub}_{K_{1,2}}(G)$.

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Lemma (see e.g. Bollobás [Bollobás 01, Corollary 2.19])

Let $d, g \geq 3$ be fixed, and dn be even. Let $\mathcal{G}_{n,d}$ denote a random d-regular graph on n vertices. Then the probability that $\mathcal{G}_{n,d}$ has girth g converges to a non-zero limit.

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$\mathcal{R}(1)$ can contain only acyclic graphs.

Proof: Assume $\exists F \in \mathcal{R}(1)$ has a cycle of length m.

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F is subgraph of $G = v(X) K_{d+1}$, but not $H = (d+1)X$ $\lightning$

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Lemma

$F \in \mathcal{R}(1) \Rightarrow F$ has no P_4 as subgraph.

Proof sketch: see Whiteboard $\longrightarrow$

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Remaining forests not in $\mathcal{C}(1)$:

F	$K_{1,2} + K_2$	$2K_{1,2}$	$K_{1,2} + 2K_2$	$3K_2$
G	C_6	C_6	C_7	C_6
$\mathrm{sub}_F(G)$	12	3	7	2
H	$2C_3$	$2C_3$	$C_4 + C_3$	C_3
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All remaining unions $F = sK_2 + tK_{1,2}$ are not in $\mathcal{C}(1)$: Take a pair G, H from above and use $G + s'K_2 + t'K_{1,2}, H + s'K_2 + t'K_{1,2}$ s.t. t' is minimal and at least one of G and H contains F.

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$\mathcal{C}(k)$

Theorem (Part of Theorem 3 in [Dell, Grohe, Rattan 18])

Let F be a graph with treewidth at most k. Then k-WL retains $\hom_F$, where $\hom_F(G)$ denotes the number of homomorphisms from F to G.

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Theorem

$\{F : \mathrm{htw}(F) \leq k\} \subseteq \mathcal{C}(k)$

Complete characterization of $\mathcal{C}(1)$ and $\mathcal{R}(1)$

Theorem (restated)

$\{F : \mathrm{htw}(F) \leq 1\} = \{K_{1,s} : s \geq 1\} \cup \{2K_2\} = \mathcal{C}(1)$.

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Proof.

K_4 is the only excluded minor for graphs of treewidth at most 3. Merging nonadjacent vertices (homomorphisms) and adjacent vertices (minors) is interchangeable. Deleting vertices (needed for minors) can be simulated by one of the other operations. □

What we know about $\mathcal{C}(2)$

Theorem

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Proof.

For $s \leq 5$, observe that $\mathrm{htw}(F)$ is at most 2 since contracting cannot increase the number of edges (to 6 for K_4). For $s \geq 6$ observe, that the rook's graph G and Shrikhande graph H are 2-WL-equivalent but contain different number of 6,7 and 8-matchings.
$G + (s-8)K_2, H + (s-8)K_2$ serve as counterexample for $s \geq 9$. □

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- This is possible if and only if K_4 has an Euler walk that is not an Euler tour (dropping the edge used twice).
- Since all vertices have odd degree, K_4 has neither of them.

□

Local counting

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$f_{\text{2-WL-local}}(G, u, v)$ retains the number of s-matchings in G that contain the edge $\{u, v\}$ if and only if $s \leq 5$.
$f_{\text{2-WL-local}}(G, u, v)$ retains the number of s-matchings in G that contain both u and v on different edges if and only if $s \leq 4$.

Outline

1. Properties, Retainment and the Weisfeiler-Lehman algorithm
2. Counting subgraphs
3. Retaining fractional graph parameters

Fractional graph parameters

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Parameter $\pi(G) \rightarrow$ IP $\overset{relaxation}{\rightarrow}$ LP $\rightarrow$ fractional parameter $\pi_f(G)$

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fractional X is a function $f : D \rightarrow [0,1]$

X	D	condition	$\lvert f \rvert$
matching	$E(G)$	$\forall x \in V(G) : \sum_{y \in N(x)} f(\{x,y\}) \leq 1$	$\sum_{e \in E(G)} f(e)$
vc	$V(G)$	$\forall \{x,y\} \in E(G) : f(x) + f(y) \geq 1$	$\sum_{x \in V(G)} f(x)$
dom. set	$V(G)$	$\forall x \in V(G) : \sum_{y \in N[x]} f(y) \geq 1$	$\sum_{x \in V(G)} f(x)$
clique	$V(G)$	$\forall I \in \mathcal{I}(G) : \sum_{x \in I} f(x) \leq 1$	$\sum_{x \in V(G)} f(x)$
coloring	$\mathcal{I}(G)$	$\forall x \in V(G) : \sum_{x \in I \in \mathcal{I}(G)} f(I) \geq 1$	$\sum_{I \in \mathcal{I}(G)} f(I)$

$\mathcal{I}(G)$ denotes the independent sets of G.

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Theorem

1-WL retains fractional matching (and thus vertex cover) and domination number. 2-WL does not retain the fractional clique (and thus chromatic) number, there are $G_s \equiv_{\text{1-WL}} H_s$, s.t. $\chi_f(G_s) = \Theta(s)$ and $\chi(H) = 2$.

Approximately retaining integral graph parameters

Known factors between integral and fractional parameters

parameter	fraction
matching n.	$\nu(G) \leq \nu_f(G) \leq \frac{3}{2}\nu(G)$[Choi, Kim, Suil 16]
vc number	$\tau_f(G) \leq \tau(G) \leq 2\tau_f(G)$[Scheinerman, Ullman 97]
	+ LP rounding
dom. number	$\frac{\gamma(G)}{\gamma_f(G)} = O(\log n)$[Chappell, Gimbel, Hartman 17]

This yields approximation ratios for these parameters retained by 1-WL. These ratios are tight (up to a constant factor for dom. number).

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