The Iteration Number of the Weisfeiler-Leman Algorithm [Grohe et al., 2023]

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1 The Weisfeiler-Leman Algorithm

The Weisfeiler-Leman (WL) algorithm is an isomorphism test. It iteratively computes an isomorphism-invariant coloring of tuples of vertices of a graph.
Two graphs are distinguished, and hence non-isomorphic, if they have different colorings. there is a well known logical characterisation:

The iteration number of k-WL, i.e., the number of iterations the algorithm requires to stabilize, this is trivially at most $n^k - 1$.

Let χ_1, χ_2: $V^k \to C$ be colorings of k-tuples over a finite set V where C is some finite set of colors. The coloring χ_1 refines χ_2, denoted $\chi_1 \preceq \chi_2$.

Let us fix $k \geq 2$ and consider a finite relational structure $\mathfrak{A}$, let $v = (v_1, \ldots, v_k) \in V^k$. We define the atomic type of v, denoted by $atp_{\mathfrak{A}}(v)$, to be the isomorphism type of the ordered substructure of $\mathfrak{A}$ induced by $\{v_1, \ldots, v_k\}$.

Next, we describe a single refinement step of k-WL. Let V be a finite set and let $\chi : V^k \to C$ be a coloring of all k-tuples over V . We define the coloring $step_k(\chi)$:

$$step_k(\chi)(v) := (\chi(v), M_\chi(v))$$

For all $v = (v_1, \ldots, v_k) \in V^k$ where $M_\chi(v) := \{\{(\chi(v[w/1]), \ldots, \chi(v[w/k]))|w \in V\}\}$ and $v[w/i] := (v_1, \ldots, v_{i-1}, w, v_{i+1}, \ldots, v_k)$ is the tuple obtained from v by replacing the i-th entry by w.

We define the initial coloring computed by k-WL on the structure $\mathfrak{A}$ via $\chi_k^{(0)}[\mathfrak{A}](v) := atp_{\mathfrak{A}}(v)$ for all $v \in (V(\mathfrak{A}))^k$.

For $r \geq 0$ we set $\chi_k^{(r+1)}[\mathfrak{A}] := step_k(\chi_k^{(r)}[\mathfrak{A}])$. Since $\chi^{(r+1)}k[\mathfrak{A}] \preceq \chi^{(r)}k[\mathfrak{A}]$ for all $r \geq 0$, there is some minimal s such that:

$$\chi_k^{(s)}[\mathfrak{A}] \equiv \chi_k^{(s+1)}[\mathfrak{A}] \equiv \chi_k^{(\infty)}[\mathfrak{A}]$$

2 Upper bound

Theorem 1. For all $k \geq 2$, the k-dimensional WL algorithm stabilizes after $O(kn^{k-1}log\, n)$ refinement rounds on all relational structures $\mathfrak{A}$ of arity at most k.

Proven for an algorithm at least as strong as WL.

- $\mathcal{P}$ a partition of V^k. $\mathcal{P}$ is compatible with equality if for all $P \in \mathcal{P}$, for all tuples $(v_1, \ldots, v_k)$, $(v'_1, \ldots, v'_k) \in P$, and all $i, j \in [k]$ it holds that:

$$v_i = v_j \text{ iff } v'_i = v'_j.$$

  This is a condition on the size of the isomorphism.

- Moreover, $\mathcal{P}$ is shufflable if for every $\pi : [k] \to [k]$ and every $P \in \mathcal{P}$ it holds that:

$$P^\pi := \{(v_{\pi(1)}, \ldots, v_{\pi(k)}) | (v_1, \ldots, v_k) \in P\} \in \mathcal{P}$$

  Stronger than permutation, also hierarchy of complexity.

The refinement process of k-WL are shufflable and compatible with equality.

Theorem 2. Let V be a finite set of size $n := |V|$, let $\chi_0 \ldots, \chi_\ell : V^k \to C$ be a sequence of colorings such that:

1. χ_t is shufflable and compatible with equality for all $t \in [0, \ell]$,
2. $step_k(\chi_{t-1}) \succeq \chi_t$ for all $t \in [\ell]$, and
3. $\chi_{t-1} \succ \chi_t$ for all $t \in [\ell]$.

Then $\ell \leq 2n^{k-1}(\lceil klog\, n\rceil + 1) = O(kn^{k-1}log\, n)$.

Note that Theorem 1 follows from Theorem 2 by observing that all colorings $\chi_k^{(i)}[\mathfrak{A}]$ obtained from the refinement process of k-WL are shufflable and compatible with equality.

3 A long sequence of stable coloring

Theorem 3. Suppose $n \geq 2k^2$ and let V be a set of size $|V| = 2n$, then there is a sequence of colorings $\chi_0 \ldots, \chi_\ell : V^k \to C$ of length $\ell \geq (\frac{n}{2k})^{k-1}$ such that:

1. χ_t is shufflable and compatible with equality for all $t \in [0, \ell]$,
2. χ_t is stable for all $t \in [0, \ell]$, and
3. $\chi_{t-1} \succ \chi_t$ for all $t \in [\ell]$.

Couple remarks on the previous theorems:

- Tight up to a factor $O(log\, n)$.
- Shows the limit of the setting, and ”parallelization arguments”.

A k-uniform set family (over U) is a collection $\mathcal{F}$ of k-element subsets of U.
From $\mathcal{F}$ on n points, we induce a coloring $\chi_{\mathcal{F}}$ on $2n$ elements, where $V = U \times \{0,1\}$, as follows:

$((u_1, a_1), \ldots, (u_k, a_k))$, $((u'_1 a'_1), \ldots, (u'_k, a'_k))$ are the same color iff:

(A) $u_i = u'_i$ for all $i \in [k]$,

(B) $(u_i, a_i) = (u_j, a_j) \Leftrightarrow (u'_i, a'_i) = (u'_j, a'_j)$ for all $i, j \in [k]$, and

(C) if $\{u_1, \ldots, u_k\} \in \mathcal{F}$, then $\sum_i a_i \equiv \sum_i a'_i \mod 2$.

Theorem 4 ([Babai and Frankl, 1988]). For every $n \geq 2k^2$ there exists a k-uniform set family $\mathcal{F}$ over a universe U of n points such that:

1. $|E_1 \cap E_2| \leq k - 2$ for all distinct $E_1, E_2 \in \mathcal{F}$, and
2. $|\mathcal{F}| \geq (\frac{n}{2k})^{k-1}$.

We set $\mathcal{F}_t := \{E_1, \ldots, E_t\}$ and $\chi_t = \chi_{\mathcal{F}_t}$, and we get stability (hard part), refinement, and compatible with equality, shufflable properties.

4 Restricted intersection problems

Definition 5. Let L be a set of nonnegative integers. The family $\mathcal{F}$ is L-intersecting, if $|E \cap F| \in L$ for every pair E, F of distinct members of $\mathcal{F}$.

Problem 6 (Restricted Intersection Problem - uniform case). Let L be a set of nonnegative integers and $k \geq 1$. What is the maximum number of members in a k-uniform L-intersecting family of subsets of a set of n elements?

Problem 7 (Restricted Intersection Problem - nonuniform case). Let L be a set of nonnegative integers. What is the maximum number of members in an L-intersecting family of subsets of a set of n elements?

Theorem 8 (Ray-Chaudhuri – Wilson Theorem). Let L be a set of s integers and $\mathcal{F}$ an L-intersecting k-uniform family of subsets of a set of n elements, where $s \leq k$. Then:

$$|\mathcal{F}| \leq \binom{n}{s}$$

Theorem 9. For every $k \geq s \geq 1$ and $n \geq 2k^2$, there exists a k-uniform family $\mathcal{F}$ of size $> (n/2k)^s$ on n points such that $|E \cap F| \leq s - 1$ for any two distinct sets $E, F \in \mathcal{F}$.

Proof. Let p be the greatest prime $\leq n/k$; this way $n/(2k) < p \leq n/k$. Fix a k-subset A of $\mathbb{F}_p$. ($k \leq p$ because $n \geq 2k^2$) Let X be an n-set containing $A \times \mathbb{F}_p$. For a function $f : A \to \mathbb{F}_p$, the graph $G(f) = \{(\xi, f(\xi)) : \xi \in A\}$ is a k-subset of X.
Our set system will consist of the graphs of the polynomials of degree $\leq s - 1$ over $\mathbb{F}_p$, restricted to A. It is easy to see that for two different polynomials of degree$\leq s - 1$, their graphs will have at most $s - 1$ points in common. The number of polynomials in question is $p^s > (n/2k)^s$.

□

References

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