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An application of intuitionistic fuzzy directed hypergraph in molecular structure representation

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Abstract: In this paper, essentially intersecting, essentially strongly intersecting, skeleton intersecting, non-trivial, sequentially simple and essentially sequentially simple Intuitionistic Fuzzy Directed Hypergraphs (IFDHGs) are defined. Also, it has been proved that if IFDHG H is ordered and essentially intersecting, then $\chi(H) \leq 3$. An IFDHG H is strongly intersecting if and only if $H^{\langle r_i, s_i \rangle}$ is intersecting for every $\langle r_i, s_i \rangle \in F(H)$ is proven and an application of IFDHG in molecular structure representation is also given.
Keywords: Intuitionistic fuzzy directed hypergraph (IFDHG), Essentially intersecting IFDHG, Molecular IFDHG of water.
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1 Introduction

The first definition of fuzzy graphs was proposed by Kaufmann, from the fuzzy relations introduced by Zadeh. Although Rosenfeld introduced another elaborated definition, including fuzzy vertex and fuzzy edges, the first definition of intuitionistic fuzzy graphs was proposed by A. Shannon and K. Atanassov [4], see also [3].

The intuitionistic fuzzy graph was defined as the set

$$G = \{\langle\langle x, y\rangle, \mu_G(x, y), \nu_G(x, y)\rangle | \langle x, y\rangle \in E_1 \times E_2\}$$

if the functions $\mu_G : E_1 \times E_2 \to [0, 1]$ and $\nu_G : E_1 \times E_2 \to [0, 1]$ define the degree of membership and the degree of non-membership, respectively, of the element $\langle x, y\rangle \in E_1 \times E_2$ to the set $G \subset E_1 \times E_2$ and for all $\langle x, y\rangle \in E_1 \times E_2 : 0 \leq \mu_G(x, y) + \nu_G(x, y) \leq 1$.

An *intuitionistic fuzzy hypergraph* (IFHG) [9] is an ordered pair $H = (V, \mathcal{E})$ where

(i) $V = \{v_1, v_2, ..., v_n\}$, is a finite set of intuitionistic fuzzy vertices,

(ii) $\mathcal{E} = \{E_1, E_2, ..., E_m\}$ is a family of crisp subsets of V,

(iii) $E_j = \{(v_i, \mu_j(v_i), \nu_j(v_j)) : \mu_j(v_i), \nu_j(v_i) \geq 0$ and $\mu_j(v_i) + \nu_j(v_i) \leq 1\}, j = 1, 2, ..., m$,

(iv) $E_j \neq \phi, j = 1, 2, ..., m$,

(v) $\bigcup_j supp(E_j) = V, j = 1, 2, ..., m$.

Here, the hyperedges E_j are crisp sets of intuitionistic fuzzy vertices, $\mu_j(v_i)$ and $\nu_j(v_i)$ denote the degrees of membership and non-membership of vertex v_i to edge E_j. Thus, the elements of the incidence matrix of IFHG are of the form $(v_{ij}, \mu_j(v_i), \nu_j(v_j))$. The sets $(V, \mathcal{E})$ are crisp sets. In [5], the intersecting IFDHG, $\mathcal{K}$-intersecting IFDHG and strongly intersecting IFDHG were studied. Here, some more intersecting concepts of fuzzy hypergraphs in [2] are extended to IFDHGs. This paper has five sections: Section 2 gives the notations which are used in this work. Section 3 deals with the definitions of IFDHG, intersecting and strongly intersecting IFDHG. In section 4, essentially intersecting, essentially strongly intersecting, skeleton intersecting, non-trivial, sequentially simple and essentially sequentially simple IFDHGs are defined. Also, it has been proved that if IFDHG H is ordered and essentially intersecting, then $\chi(H) \leq 3$. An IFDHG H is strongly intersecting if and only if $H^{\langle r_i, s_i\rangle}$ is intersecting for every $\langle r_i, s_i\rangle \in F(H)$ is proven and an application of IFDHG in molecular structure representation is also given. Section 5 gives the conclusion of this paper.

2 Notations

The notations used in this work are listed below:

$H = (V, \mathcal{E})$	– IFDHG with vertex set V and edge set $\mathcal{E}$
$\langle\mu_i, \nu_i\rangle$	– degrees of membership and non-membership of the vertex v_i
$\langle\mu_{ij}, \nu_{ij}\rangle$	– degrees of membership and non-membership of the i^{th} vertex in j^{th} edge
$\langle\mu_{ij}(v_i), \nu_{ij}(v_i)\rangle$	– degrees of membership and non-membership of the edges containing v_i
$h(H)$	– height of a hypergraph H
$F(H)$	– Fundamental sequence of H
$Tr(H)$	– Intuitionistic Fuzzy Transversals (IFT) of H
$C(H)$	– Core set of H

$H^{\langle r_i,s_i\rangle}$	– $\langle r_i, s_i\rangle$-level of H
$\mathcal{IF}_p(V)$	– Intuitionistic Fuzzy power set of V.
$\widetilde{E}_j$	– spike reduction of $E_j \in \mathcal{IF}_p(V)$
ϕ	– empty IFS (i.e., IFS having elements with zero membership and unit non-membership values).

3 Prerequisites

In this section, the basic definitions relating to intuitionistic fuzzy directed hypergraphs are given.

Definition 3.1. [10] An *intuitionistic fuzzy directed hypergraph* (IFDHG) H is a pair $(V, \mathcal{E})$, where V is a non empty set of vertices and $\mathcal{E}$ is a set of intuitionistic fuzzy hyperarcs; an intuitionistic fuzzy hyperarc $E_i \in \mathcal{E}$ is defined as a pair $(tl\,(E_i)\,, hd\,(E_i))$, where $tl\,(E_i) \subset V$, with $tl\,(E_i) \neq \emptyset$, is its tail, and $hd\,(E_i) \in V - tl\,(E_i)$ is its head. A vertex s is said to be a *source vertex* in H if $hd\,(E_i) \neq s$, for every $E_i \in \mathcal{E}$. A vertex d is said to be a *destination vertex* in H if $d \neq tl\,(E_i)$, for every $E_i \in \mathcal{E}$.

Definition 3.2. [5] An intuitionistic fuzzy directed hypergraph is said to be *elementary* if $\mu_{ij} : V \to [0,1]$ and $\nu_{ij} : V \to [0,1]$ are constant functions or has a range $\{0, a\}, a \neq 0$. If $|supp(\mu_{ij}, \nu_{ij})| = 1$, then it is called a *spike*. That is, an intuitionistic fuzzy subsets with singleton support.

Definition 3.3. [5] Let $H = (V, \mathcal{E})$ be an intuitionistic fuzzy directed hypergraph and $C(H) = \{H^{\langle r_1,s_1\rangle}, H^{\langle r_2,s_2\rangle}, ...H^{\langle r_n,s_n\rangle}\}$. H is said to be *ordered* if $C(H)$ is ordered. That is $H^{\langle r_1,s_1\rangle} \subset H^{\langle r_2,s_2\rangle} \subset ... \subset H^{\langle r_n,s_n\rangle}$. The intuitionistic fuzzy directed hypergraph is said to be *simply ordered* if the sequence $\{H^{\langle r_i,s_i\rangle}/i = 1, 2, 3..., n\}$ is simply ordered. That is, if H is ordered and if whenever $E \in H^{\langle r_{i+1},s_{i+1}\rangle} - H^{\langle r_i,s_i\rangle}$ then $E \not\subseteq H^{\langle r_i,s_i\rangle}$.

Definition 3.4. [7] Let H be an IFDHG. A *primitive p-coloring* A of H is a partition $\{A_1, A_2, A_3, ..., A_p\}$ of V into p-subsets (colors) such that the support of each intuitionistic fuzzy hyperedge of H intersects atleast two colors of A, except spike edges.

Definition 3.5. [7] Let H be an IFDHG. Let $C(H) = \{H^{\langle r_1,s_1\rangle}, H^{\langle r_2,s_2\rangle}, ..., H^{\langle r_n,s_n\rangle}\}$. A $\mathcal{K}$*-coloring* A of H is a partition $\{A_1, A_2, A_3, ...A_p\}$ of V into p-subsets (colors) such that A induces a coloring for each core hypergraph $H^{\langle r_i,s_i\rangle}$ of H with $H^{\langle r_i,s_i\rangle} = (V_i, \mathcal{E}_i)$ where $V_i \subset V$ and $\mathcal{E}_i \subset \mathcal{E}$. The restriction of A to V_i, $\{A_1 \cap V_i, A_2 \cap V_i, A_3 \cap V_i, ...A_k \cap V_i\}$, is coloring of $\{H^{\langle r_i,s_i\rangle}\}$. (Allow color set A_i to be empty).

Definition 3.6. [7] The *p-chromatic number* of an IFDHG H is the minimal number $\chi_p(H)$, of colors needed to produce a primitive coloring of H. The *chromatic number* of H is the minimal number, $\chi(H)$, of colors needed to produce a $\mathcal{K}$-coloring of H.

Definition 3.7. [5] An IFDHG $H = (V, \mathcal{E})$ is support simple if whenever $E_j, E_k \in \mathcal{E}, E_j \subseteq E_k$ and $supp(E_j) = supp(E_k)$ then $E_j = E_k$ for all j and k.

Definition 3.8. [5] An intuitionistic fuzzy directed hypergraph $H = (V, \mathcal{E})$ is called (μ,ν)-*tempered* intuitionistic fuzzy directed hypergraph (TIFDHG), if there exists intuitionistic fuzzy subsets $\mu_{ij} : V \to [0,1]$ and $\nu_{ij} : V \to [0,1]$ such that $\mathcal{E} = \{(\mu_{ij}(v_i), \nu_{ij}(v_i))/v_i \in E_j\}$ where

$$\mu_{ij}(v_i) = \begin{cases} \wedge\mu_j(y)/y \in E_j & \text{if } v_i \in E_j \\ 0 & \text{otherwise} \end{cases}, \quad \text{and} \quad \nu_{ij}(v_i) = \begin{cases} \vee\{\nu_i(y)/y \in E_j & \text{if } v_i \in E_j \\ 0 & \text{otherwise} \end{cases},$$

for every v_i, $0 < \mu_{ij}(v_i) + \nu_{ij}(v_i) \leq 1$.

Definition 3.9. [5] A *minimal intuitionistic fuzzy transversal* T for H is a transversal of H with the property that if $T_1 \subset T$, then T_1 is not an intuitionistic fuzzy transversal of H.

Definition 3.10. [6] An IFDHG $H = (V, \mathcal{E})$ is said to be *intersecting intuitionistic fuzzy directed hypergraph*, if for each pair of intuitionistic fuzzy hyperedge $E_i, E_j \in \mathcal{E}, E_i \bigcap E_j \neq \phi$ where ϕ is an IFS whose elements have zero membership and unit non-membership values.

Definition 3.11. [6] An IFDHG H is said to be *strongly intersecting*, if for any two edges E_i and E_j contain a common spike of height, $h = h(E_i) \wedge h(E_j)$.

Definition 3.12. [6] Let H be an IFDHG and $C(H) = \{H^{\langle r_1,s_1\rangle}, H^{\langle r_2,s_2\rangle}, ..., H^{\langle r_n,s_n\rangle}\}$, if $H^{\langle r_i,s_i\rangle}$ is an intersecting IFDHG for each $i = 1, 2, ..., n$ then H is $\mathcal{K}$-*intersecting IFDHG*.

Definition 3.13. [12] The *Intuitionistic fuzzy triangular function (iftrif)*, is specified by three parameters, a lower limit a, an upper limit c, and a value b, where $a \leq b \leq c$. Intuitionistic fuzzy triangular membership function and non-membership function of A takes the form

$$\mu_A(x) = \begin{cases} 0 & ; \ x \leq a \\ (\frac{x-a}{b-a}) - \epsilon & ; \ a < x \leq b \\ (\frac{c-x}{c-b}) - \epsilon & ; \ b \leq x < c \\ 0 & ; \ x \geq c \end{cases}, \qquad \nu_A(x) = \begin{cases} 1-\epsilon & ; \ x \leq a \\ 1-(\frac{x-a}{b-a}) & ; \ a < x \leq b \\ 1-(\frac{c-x}{c-b}) & ; \ b \leq x < c \\ 1-\epsilon & ; \ x \geq c \end{cases}$$

Theorem 3.1. [6] Let H be an IFDHG. Then H is strongly intersecting if and only if H is $\mathcal{K}$-intersecting.

4 Intersecting intuitionistic fuzzy directed hypergraphs

In this section, essentially intersecting, essentially strongly intersecting, skeleton intersecting, non-trivial, sequentially simple and essentially sequentially simple IFDHGs are defined.

4.1 Essentially intersecting IFDHGs

Definition 4.1. A spike reduction of $E_j \in \mathcal{IF}_p(V)$, denoted by $\widetilde{E_j}$, is defined by

$$\widetilde{E_j}^{\langle r_j,s_j\rangle} = \begin{cases} E_j^{\langle r_j,s_j\rangle} & \text{if } \ |E_j^{\langle r_j,s_j\rangle}| \geq 2 \\ \phi & \text{if } \ |E_j^{\langle r_j,s_j\rangle}| < 2 \end{cases}$$

where $r_j = \min\{\mu_j(v_i)\} \in (0,1]$ and $s_j = \max\{\nu_j(v_i)\} \in [0,1)$

Definition 4.2. Let $H = (V, \mathcal{E})$ be an IFDHG. The spike reduced IFDHG of H, denoted by $\widetilde{H}$, is defined as $\widetilde{H} = (\widetilde{V}, \widetilde{\mathcal{E}})$, where $\widetilde{\mathcal{E}} = \{\widetilde{E_j} | E_j \in \mathcal{E}\}$; $\widetilde{V} = \bigcup_{\widetilde{E_j} \in \widetilde{\mathcal{E}}} supp(\widetilde{\mathcal{E}})$ and

$$\langle \mu_j(\widetilde{v_i}), \nu_j(\widetilde{v_i}) \rangle = \begin{cases} \langle r_j, s_j \rangle & \text{if } \widetilde{v_i} \in supp(\widetilde{E_j}) \\ \langle 0, 1 \rangle & \text{if } \widetilde{v_i} \notin supp(\widetilde{E_j}) \end{cases}$$

Example 1. Consider an IFDHG H with $V = \{v_1, v_2, v_3, v_4, v_5\}$ and $\mathcal{E} = \{E_1, E_2, E_3, E_4\}$ whose incidence matrix as follows:

$$H = \begin{array}{c} \\ v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \end{array} \begin{array}{c} \begin{array}{cccc} E_1 & E_2 & E_3 & E_4 \end{array} \\ \begin{pmatrix} \langle 0.8, 0.1 \rangle & \langle 0, 1 \rangle & \langle 0, 1 \rangle & \langle 0, 1 \rangle \\ \langle 0.6, 0.2 \rangle & \langle 0.5, 0.2 \rangle & \langle 0, 1 \rangle & \langle 0, 1 \rangle \\ \langle 0, 1 \rangle & \langle 0.8, 0.1 \rangle & \langle 0.3, 0.4 \rangle & \langle 0, 1 \rangle \\ \langle 0.3, 0.6 \rangle & \langle 0, 1 \rangle & \langle 0.6, 0.2 \rangle & \langle 0, 1 \rangle \\ \langle 0, 1 \rangle & \langle 0, 1 \rangle & \langle 0, 1 \rangle & \langle 0.5, 0.1 \rangle \end{pmatrix} \end{array}$$

Then the incidence matrix of $\widetilde{H} = (\widetilde{V}, \widetilde{\mathcal{E}})$, where $\widetilde{\mathcal{E}} = \{\widetilde{E}_1, \widetilde{E}_2, \widetilde{E}_3\}$ and $\widetilde{V} = \{\widetilde{v}_1, \widetilde{v}_2, \widetilde{v}_3, \widetilde{v}_4, \widetilde{v}_5\}$ is as follows:

$$\widetilde{H} = \begin{array}{c} \\ \widetilde{v}_1 \\ \widetilde{v}_2 \\ \widetilde{v}_3 \\ \widetilde{v}_4 \\ \widetilde{v}_5 \end{array} \begin{array}{c} \begin{array}{ccc} \widetilde{E}_1 & \widetilde{E}_2 & \widetilde{E}_3 \end{array} \\ \begin{pmatrix} \langle 0.3, 0.6 \rangle & \langle 0, 1 \rangle & \langle 0, 1 \rangle \\ \langle 0.3, 0.6 \rangle & \langle 0.5, 0.2 \rangle & \langle 0, 1 \rangle \\ \langle 0, 1 \rangle & \langle 0.5, 0.2 \rangle & \langle 0.3, 0.4 \rangle \\ \langle 0.3, 0.6 \rangle & \langle 0, 1 \rangle & \langle 0.3, 0.4 \rangle \\ \langle 0, 1 \rangle & \langle 0, 1 \rangle & \langle 0, 1 \rangle \end{pmatrix} \end{array}$$

Note: It is to be noted that there are two changes happened in $\widetilde{H}$:

(i) The spike is reduced;

(ii) The degrees of membership and nonmembership of the vertices have been modified.

The graphs of H and $\widetilde{H}$ are given in Figure 1.

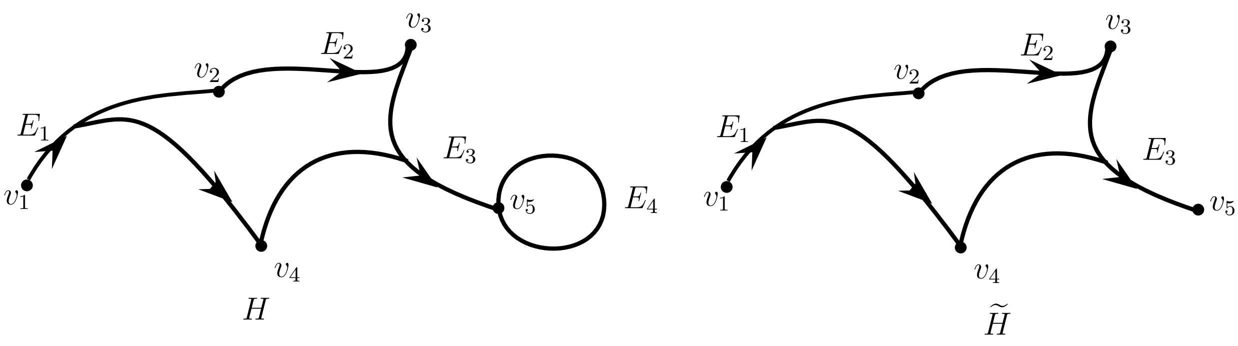


Figure 1

Definition 4.3. A IFDHG H is said to be *essentially intersecting* if $\widetilde{H}$ is intersecting. H is said to be *essentially strongly intersecting* if $\widetilde{H}$ is strongly intersecting.

Theorem 4.1. If IFDHG H is ordered and essentially intersecting, Then $\chi(H) \leq 3$.

Proof. Assume that $\widetilde{H}$ exists, for otherwise $\chi(H)$=1. Let $(\widetilde{H})^{\langle r_m, s_m \rangle} \in C(\widetilde{H})$, where $\langle r_m, s_m \rangle$ is the smallest value of $F(\widetilde{H})$. Since $\widetilde{H}$ is intersecting, it follows from known theorem *"Let H be an IFDHG and suppose $C(H) = \{H^{\langle r_1,s_1 \rangle}, H^{\langle r_2,s_2 \rangle}, ..., H^{\langle r_n,s_n \rangle}\}$, then H is intersecting if and only if $H^{\langle r_n,s_n \rangle} = (V^{\langle r_n,s_n \rangle}, \mathcal{E}^{\langle r_n,s_n \rangle})$ is intersecting"* that $(\widetilde{H})^{\langle r_m,s_m \rangle}$ is a crisp intersecting hypergraph. Therefore, $\chi(\widetilde{H})^{\langle r_m,s_m \rangle} \leq 3$ since *"If H is a crisp intersecting hypergraph, then $\chi(H) \leq 3$."*

Since H is ordered, $\widetilde{H}$ is also ordered. A coloring of $(\widetilde{H})^{\langle r_m,s_m \rangle}$ must be a primitive coloring of $\widetilde{H}$ (Definition 3.4), it follows from known theorem *"If H is an ordered IFDHG and A is a primitive coloring of H, then A is a $\mathcal{K}$-coloring of H"* that a coloring of $(\widetilde{H})^{\langle r_m,s_m \rangle}$ is a $\mathcal{K}$-coloring of $\widetilde{H}$. Therefore, $\chi(\widetilde{H}) \leq 3$ implies that $\chi(H) \leq 3$. □

Corollary 4.2. If IFDHG H is elementary and essentially intersecting, then $\chi(H) \leq 3$.

Corollary 4.3. If H is (μ, ν)-tempered IFDHG and essentially intersecting, then $\chi(H) \leq 3$.

Definition 4.4. An IFDHG is said to be *non-trivial* if it has at least one edge E such that $|supp(E)| \geq 2$.

Definition 4.5. An IFDHG H is said to be *sequentially simple* if

$$C(H) = \{H^{\langle r_i,s_i \rangle} = (X^{\langle r_i,s_i \rangle}, \mathcal{E}^{\langle r_i,s_i \rangle}) | \langle r_i, s_i \rangle \in F(H)\}$$

satisfies the property that if $E \in \mathcal{E}^{\langle r_{i+1},s_{i+1} \rangle} \setminus \mathcal{E}^{\langle r_i,s_i \rangle}$, then $E \nsubseteq X^{\langle r_i,s_i \rangle}$, where $r_n < ... < r_1$, $s_n < ... < s_1$. H is said to be *essentially sequentially simple* if $\widetilde{H}$ is sequentially simple.

Definition 4.6. Suppose $H = \{E_i \in \mathcal{IF}_p(V) | i = 1, 2, 3, ..., m\}$ is a finite collection of intuitionistic fuzzy subsets of V and let $r, s \in (0, 1]$. Then $H|_{\langle r,s \rangle} = \{E \in \mathcal{IF}_p(V) | h(E) = \langle r, s \rangle\}$ is the set of edges of height $\langle r, s \rangle$. In particular, $H|_{\langle r,s \rangle}$ is the partial directed hypergraph of $H = (V, \mathcal{E})$ with edgeset $\mathcal{E}|_{\langle r,s \rangle}$, provided $\mathcal{E}|_{\langle r,s \rangle} \neq \phi$.

Definition 4.7. Let $H_i = (X_i, \mathcal{E}_i), i = 1, 2$ be IFDHGs. Then $H_1 \preceq H_2$ if every edge of H_1 contains an edge of H_2.

Theorem 4.4. An IFDHG H is strongly intersecting if and only if $H^{\langle r_i,s_i \rangle} \preceq Tr(H^{\langle r_i,s_i \rangle})$ for every $H^{\langle r_i,s_i \rangle} \in C(H)$.

Proof. By Theorem 3.1, Definition 3.12 and known lemma "A crisp hypergraph H is intersecting if and only if $H \preceq Tr(H)$", H is strongly intersecting. $\Leftrightarrow$ H is $\mathcal{K}$-intersecting. $\Leftrightarrow$ $H^{\langle r_i,s_i \rangle}$ is intersecting for all $H^{\langle r_i,s_i \rangle} \in C(H) \Leftrightarrow H^{\langle r_i,s_i \rangle} \preceq Tr(H^{\langle r_i,s_i \rangle})$ for all $H^{\langle r_i,s_i \rangle} \in C(H)$. □

Theorem 4.5. H is a strongly intersecting IFDHG if and only if for every $\langle r_i, s_i \rangle \in F(H)$, $(H^{\langle r_i,s_i \rangle})|_{\langle r_i,s_i \rangle} \preceq Tr(H^{\langle r_i,s_i \rangle})$.

Proof. Suppose for every $\langle r_i, s_i\rangle \in F(H)$, $(H^{\langle r_i,s_i\rangle})|_{\langle r_i,s_i\rangle} \preceq Tr(H^{\langle r_i,s_i\rangle})$. For each $H^{\langle r_i,s_i\rangle} \in C(H)$, the edge set $E(H^{\langle r_i,s_i\rangle}) = \{\gamma^{\langle r_i,s_i\rangle}|\gamma \in (H^{\langle r_i,s_i\rangle})|_{\langle r_i,s_i\rangle} \preceq \{\tau^{\langle r_i,s_i\rangle}|\tau \in Tr(H^{\langle r_i,s_i\rangle})\} = Tr(E(H^{\langle r_i,s_i\rangle}))$. Hence, $H^{\langle r_i,s_i\rangle} \preceq Tr(H^{\langle r_i,s_i\rangle})$, for every $H^{\langle r_i,s_i\rangle} \in C(H)$ and by Theorem 4.5, H is strongly intersecting.

Conversely, suppose H is strongly intersecting. Let $\gamma \in H|_{\langle r_1,s_1\rangle}$, where $\langle r_1, s_1\rangle$ is the largest member of $F(H)$. Let $H^{\langle r_j,s_j\rangle} \in C(H)$. To show that $\gamma^{\langle r_j,s_j\rangle}$ is a transversal of $H^{\langle r_j,s_j\rangle}$ For suppose $E \in H^{\langle r_j,s_j\rangle}$. Then there is an edge η of H such that $\eta^{\langle r_j,s_j\rangle} = E$. Since H is strongly intersecting, there is a spike σ_x such that $h(\sigma_x) = h(\gamma) \wedge h(\eta) = h(\eta) \geq \langle r_j, s_j\rangle$, and support $\{x\}$, which is contained in both γ and η.

Hence, $x \in E \cap \alpha^{\langle r_j,s_j\rangle}$. Thus, γ is a transversal of H and therefore contains a member of $Tr(H)$. Therefore, $(H^{\langle r_i,s_i\rangle})|_{\langle r_i,s_i\rangle} \preceq Tr(H^{\langle r_1,s_1\rangle})$. Using Theorem 3.1, H is $\mathcal{K}$-intersecting. Consequently, by Theorem 3.1, it follows that $H^{\langle r_i,s_i\rangle}$ must be strongly intersecting. Hence $(H^{r_i,s_i})|_{\langle r_i,s_i\rangle} \preceq Tr(H^{\langle r_i,s_i\rangle})$, for each $\langle r_i, s_i\rangle \in F(H)$. □

Corollary 4.6. Let H be an IFDHG with $C(H) = \{H^{\langle r_i,s_i\rangle}|\langle r_i, s_i\rangle \in F(H)\}$. Then $H^{\langle r_i,s_i\rangle} \preceq Tr(H^{\langle r_i,s_i\rangle})$, for every $H^{r_i,s_i} \in C(H)$ if and only if $(H^{r_i,s_i})|_{\langle r_i,s_i\rangle} \preceq Tr(H^{\langle r_i,s_i\rangle})$, for every $\langle r_i, s_i\rangle \in F(H)$.

Theorem 4.7. An IFDHG H is strongly intersecting if and only if $H^{\langle r_i,s_i\rangle}$ is intersecting for every $\langle r_i, s_i\rangle \in F(H)$.

Proof. By applying the Theorem, *"Let H be an IFDHG and suppose*

$$C(H) = \left\{H^{\langle r_1,s_1\rangle}, H^{\langle r_2,s_2\rangle}, ..., H^{\langle r_n,s_n\rangle}\right\}.$$

Then H is intersecting if and only if $H^{\langle r_n,s_n\rangle} = (V^{\langle r_n,s_n\rangle}, \mathcal{E}^{\langle r_n,s_n\rangle})$ is intersecting" to $H^{\langle r_i,s_i\rangle}$, and by Theorem 3.1, $H^{\langle r_i,s_i\rangle}$ is intersecting for every $\langle r_i, s_i\rangle \in F(H) \Leftrightarrow E(H^{\langle r_i,s_i\rangle})$ is intersecting for each $H^{\langle r_i,s_i\rangle} \in C(H) \Leftrightarrow H$ is $\mathcal{K}$-intersecting $\Leftrightarrow H$ is strongly intersecting. □

4.2 Application of IFDHG in chemistry

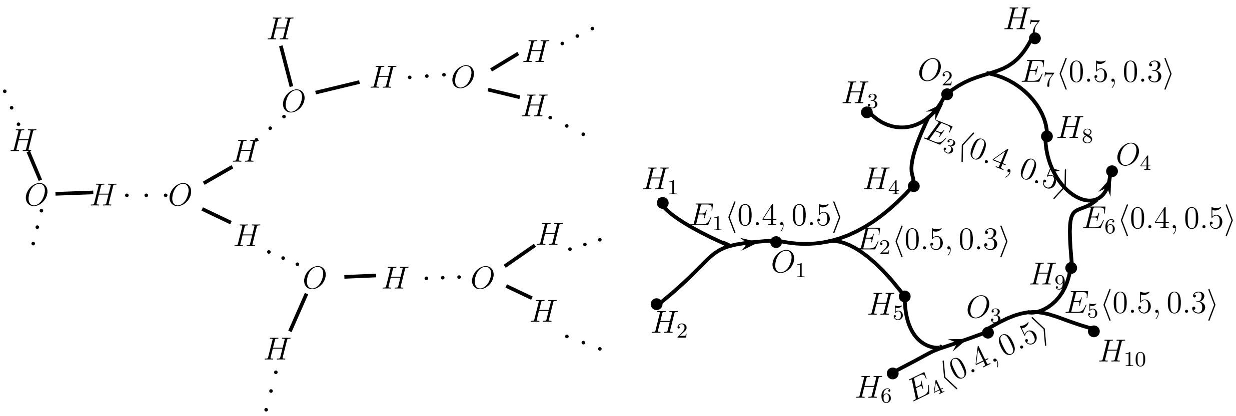
Chemical compounds are formed by the joining of two or more atoms. A *chemical bond* is a lasting attraction between atoms that enables the formation of chemical compounds [11]. There are two major chemical bond classifications namely Primary (Strong) bonds and Secondary (Weak) bonds each with identifiable subgroups as ionic, covalent, metallic and hydrogen, Van der Waal's bonds respectively.

The power of an atom in a molecule to attract electrons to itself is called *electronegativity*. Covalent bonds are formed when the electronegativity difference (D^c) between the atoms is < 1.7. Ionic bonds are formed when the electronegativity difference (D^c) between the atoms is > 1.7. Based on Pauling scale for Electronegativity, Carbon (C) atom has electonegativity 2.5, Oxygen (O) has 3.5 and Hydrogen (H) has electronegativity 2.1.

Bond length is the distance between centers of atoms bonded within a molecule. Bond length depends on three main factors such as size of atoms, bond strength and multiplicity of bonds. Also, the temperature and pressure affect the bondlength between atoms and hence, uncertainty exists in the molecular structure. therefore, the concept of IFDHG can also be used as a tool to deal this kind of uncertainity.

An IFDHG $H = (V, \mathcal{E})$ is used to represent molecular structure, where $x \in V$ corresponds to an atom, intuitionistic fuzzy directed hyperedges correspond to bonds between the atoms. Such IFDHGs are known as molecular IFDHGs. The directions of intuitionistic fuzzy hyperedges represent the direction towards the atom which has more electronegativity. Membership amd non-membership values of the intuitionistic fuzzy hyperedges depends on the length of the bonds between the atom. Bond length depends on bond order between atoms, electronegativity force of the atoms and intermolecular forces between the molecules.

In Figure 2 (a), the molecular structure of water is shown. Here, the dotted lines represent the hydrogen bonds between the Oxygen and Hydrogen atoms, remaining are covalent bonds. In Figure 2 (b), molecular IFDHG representation of water is shown. In this molecular IFDHG, the directions represent the direction towards the atom which has more electronegativity. Intuitionistic fuzzy directed hyperedge E_1 connect two Hydrogen atoms with an Oxygen atom. Oxygen atom has more eletronegativity than the Hydrogen atom. So the $hd(E_1)$ is Oxygen atom and two hydrogen atoms are $tl(E_1)$.



(a) Molecular structure of water

(b) Molecular IFDHG of water

Figure 2

The membership and non-membership values of $E_i, i = 1, ..., 7$ is denoted by $\langle \mu(E_i), \nu(E_i)\rangle$. The bond length of the covalent bond between Hydrogen and Oxygen atoms is $0.96A^0$ (Angstrom) and hydrogen bond length between these two atoms is $1.97A^0$ (Angstrom).

In Definition 3.13, let $a = 0.5, b = 1.5$ and $c = 3.0, x = 0.96$ (Bond length). Therefore, $\langle \mu(E_i), \nu(E_i)\rangle = \langle 0.4, 0.5\rangle$ for $i = 1, 3, 4$ and 6. In a similar way, the membership and non-membership values of intuitionistic fuzzy hyperedges are calculated.

5 Conclusion

In this paper, an attempt has been made to define essentially intersecting, essentially strongly intersecting, skeleton intersecting, non-trivial, sequentially simple and essentially sequentially simple IFDHG. Also an application of IFDHGs in molecular structure representation has been given. As this is an initiative taken to represent molecular structures using IFDHGs, the authors further proposed to apply the properties of IFDHGs to study and compare the properties of molecular structures of all states of water.

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