Polynomial time vertex enumeration of convex polytopes of bounded branch-width

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Outline

Vertex enumeration

Given polytope by its outer description
$P = \{x \in \mathbb{R}^{\mathcal{N}} \mid Sx = b, x \geq 0\}$
enumerate all its vertices

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Can this be done in total polynomial time?
Time polynomial in size of input and output

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Most popular method: Double Description method [Fukuda] or more sophisticated [Terzer & Stelling 08]

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Branch-decomposition and branch width defined for matroids

Our result: For $P = \{x \in \mathbb{R}^{\mathcal{N}} \mid Sx = b, x \geq 0\}$, if the branch-width of the linear matroid on the columns of S is bounded by k, then we can enumerate all vertices $\mathcal{V}$ in running time $O(\mathcal{N}|\mathcal{V}|^{O(k)}t)$, where t is time for solving some LP's for feasibility checks

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- Network of chemical reactions
  together performing some constructive and destructive tasks in a living cell
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- Each reaction gives a column of the stoichiometric matrix

Stougiometric Matrix

Example: $1NH_3+2O_2 \rightarrow 1HNO_3+1H_2O$

	R
·	0
·	0
NH_3	-1
O_2	-2
HNO_3	$+1$
H_2O	$+1$
·	0
·	0

Flux

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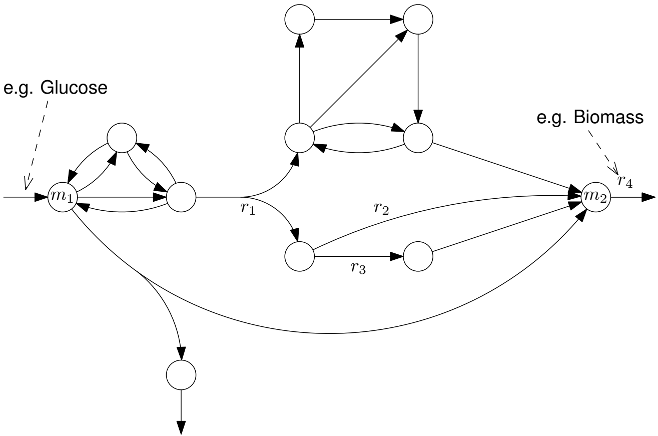
- Steady state assumption

$$Sv = 0, v \geq 0$$

Running Example



Here all coefficients of the stoichiometric matrix are $-1, 0, +1$.

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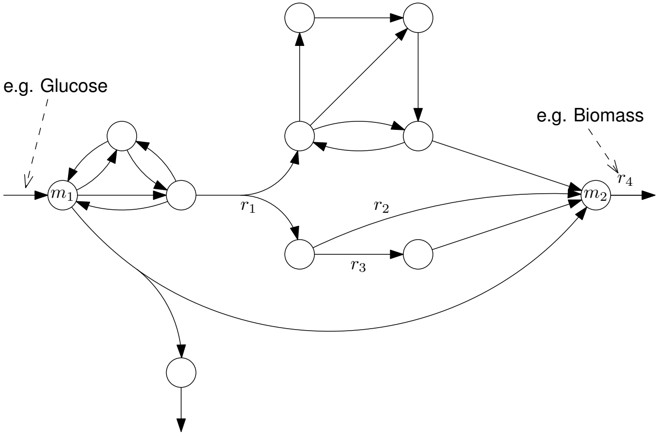

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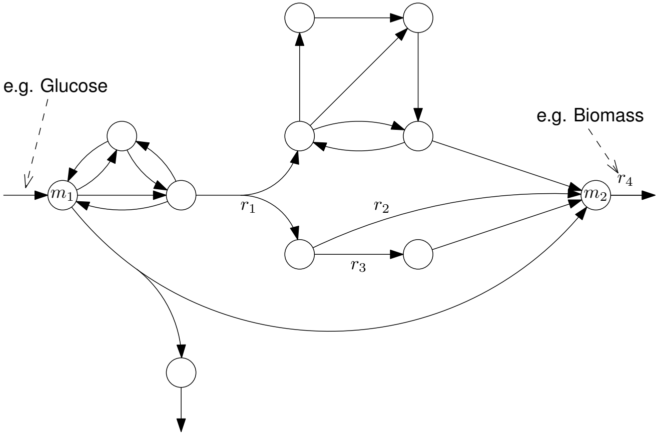

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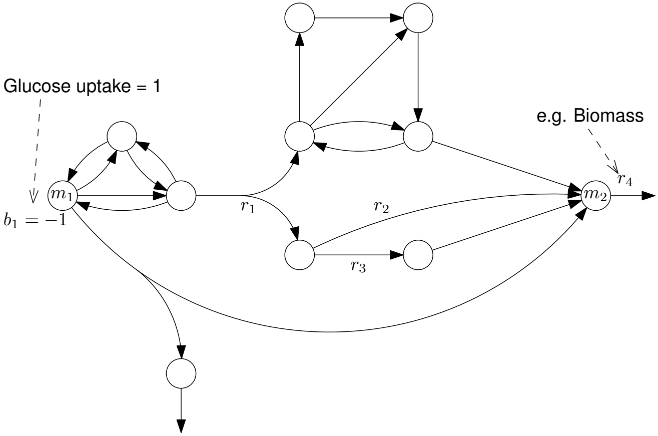

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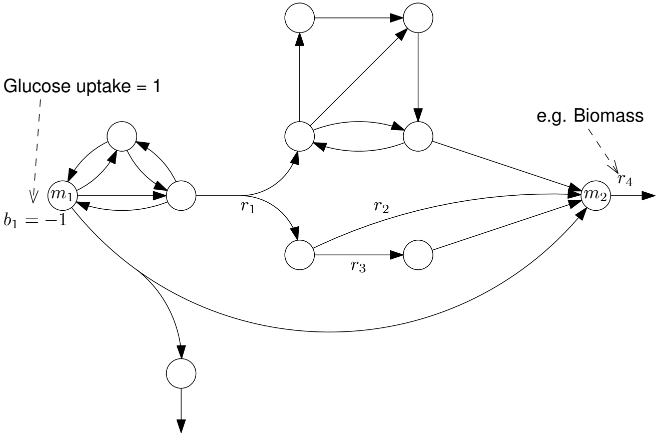

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- Optimize Biomass production (linear programming)

$$\max v_{biomass} \quad \text{subject to } Sv = 0, \; v_{glucose} = 1$$

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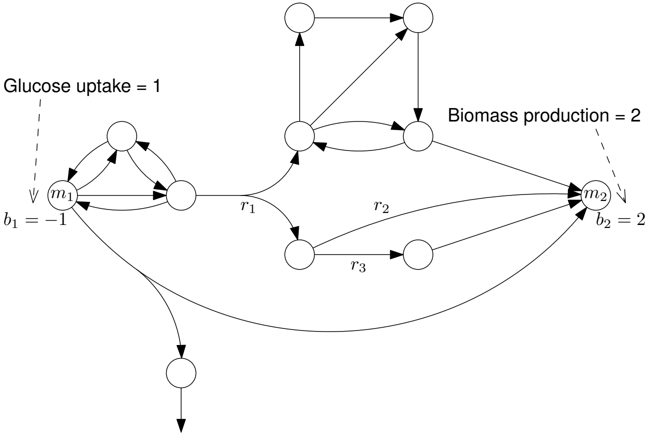

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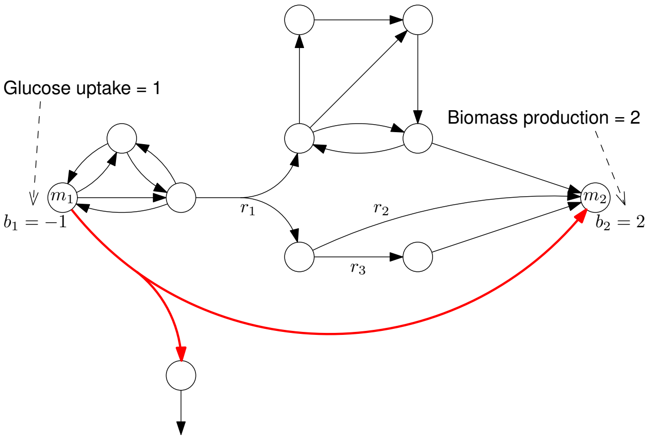

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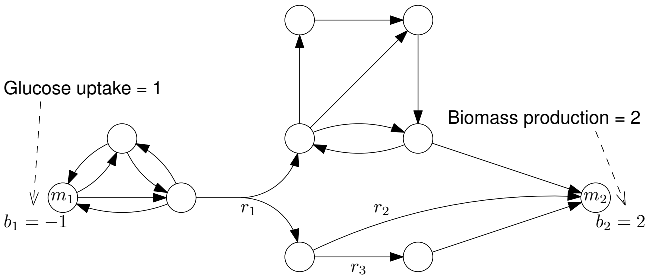

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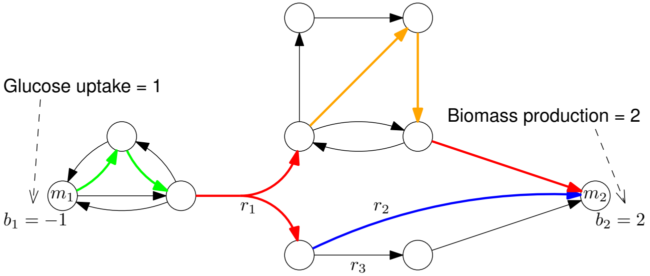

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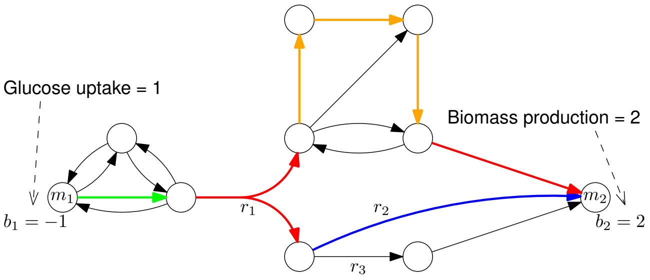

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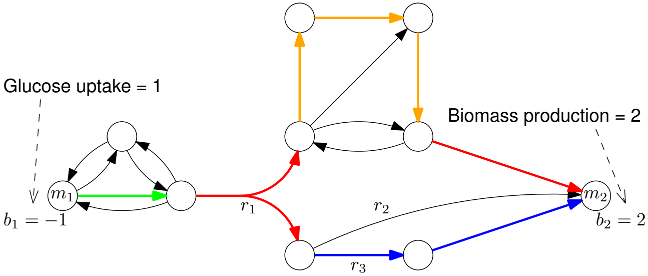

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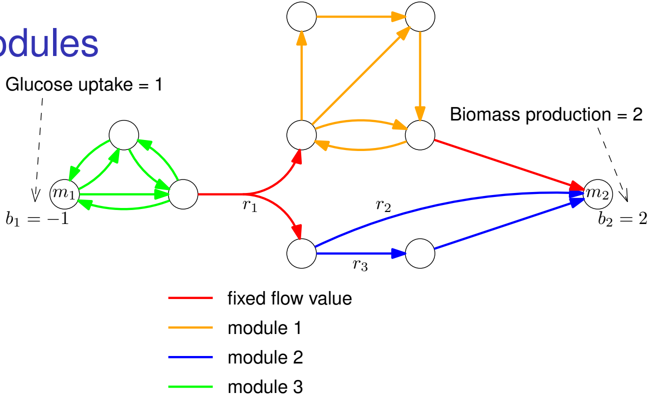
Flux-Modules



Observation (Kelk, Olivier, S., Bruggeman ’12)

Reaction rates in the green module are independent from reaction rates in the orange module are independent from reaction rates in the blue module.

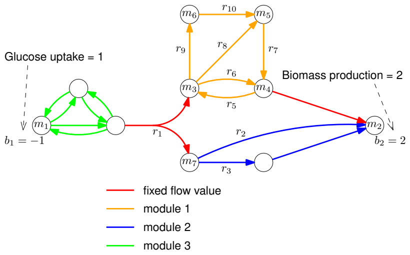
Kelk et al., Optimal flux spaces of genome-scale stoichiometric models are determined by a few subnetworks *Nature Scientific Reports*, 2:580, 2012.

Flux-Modules: A Definition

Notation:

- $\mathcal{N}$ reactions (variables, columns)
- $\mathcal{M}$ metabolites (constraints, rows)
- S stoichiometric matrix
- $P \subseteq \mathbb{R}^{\mathcal{N}}$ flux space: In Ex.

$\{v : Sv = 0, v_{glucose} = 1, v_{biomass} = 2, v \geq 0\}$



Definition (Reimers '13)

$A \subseteq \mathcal{N}$ is a P-module if $\exists d \in \mathbb{R}^{\mathcal{M}}$ s.t. $S_A v_A = d$ for all $v \in P$.

- A module is a set of reactions A.
- The interface flux $d = S_A v_A$ of a module is constant for all feasible flux vectors ($v \in P$).

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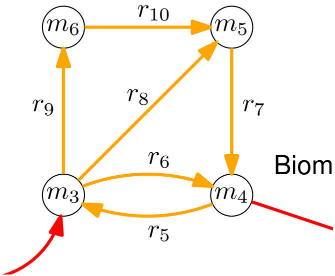

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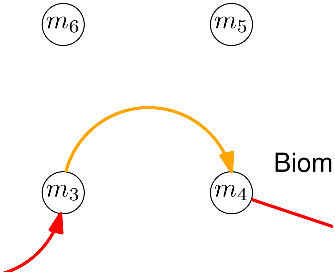

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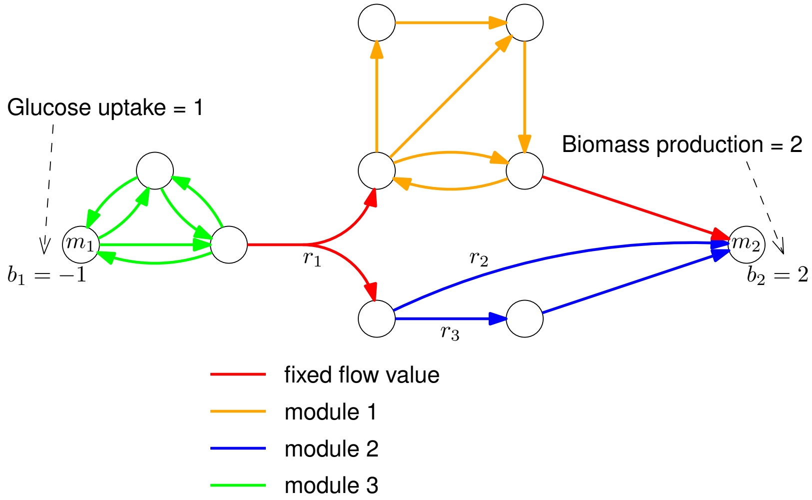
Decomposition of Elementary Flux Modes (EFM)

A graphical visualization of all 12 EFMs in the example network



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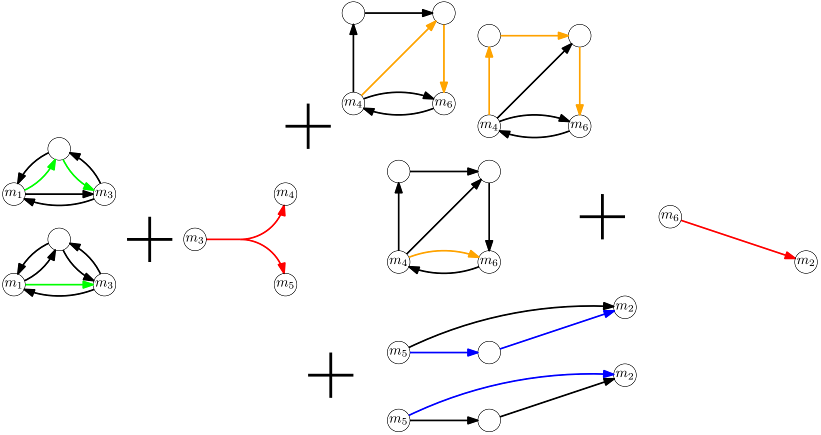

Outline

k-modules

Definition (module)

$A \subseteq \mathcal{N}$ is a module of P if there exists a $d \in \mathbb{R}^{\mathcal{M}}$, s.t. for all $x \in P$

$$S_A x_A = d \qquad .$$

k-modules

Definition (k-module)

$A \subseteq \mathcal{N}$ is a k-module of P if there exists a $d \in \mathbb{R}^{\mathcal{M}}$, $D \in \mathbb{R}^{\mathcal{M} \times k}$ s.t. for all $x \in P$ exists a $\alpha \in \mathbb{R}^k$ with

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If $d = 0$ we call A a linear k-module

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- k-modules relate to k-separations of the matroid with ground set the columns of the constraint matrix

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A is a k-module for P $\Leftrightarrow$ A is a k-module for ker(S)

Under the condition that no x_i has fixed value on P
which can be ensured by preprocessing if necessary.

k-modules and Matroids

Definition (*k*-separator, Oxley 2011)

Let M be a matroid on the element set $\mathcal{N}$. A set $A \subseteq \mathcal{N}$ is a k-separator if and only if

$$\mathrm{rank}(A) + \mathrm{rank}(\mathcal{N} \setminus A) - \mathrm{rank}(\mathcal{N}) < k.$$

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Separation is a measure of connectivity of the matroid

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Theorem

$A \subseteq \mathcal{N}$ is a $(\ker S)$-k-module if and only if A is a $k+1$-separator in the linear matroid M represented by S.

Branch Decomposition of columns of S

Definition (branch-width)

- A *branch decomposition* (T, τ) consists of a tree T with nodes of degree 3 and 1 and a bijective map $\tau : T \to \mathcal{N}$. Define $\tau(A) := \{\tau(a) : a \in A\}$.
- The *width* of edge e of T is $\rho(\tau(A_e))$, where (A_e, B_e) the partition of the leaves of T given by $T \setminus e$. (Note that $\rho(A) = \rho(\mathcal{N} \setminus A)$.)
- The width of a branch decomposition is the maximal width of an edge $e \in T$.
- The *branch-width* of M is the minimal width of all possible branch-decompositions.

With connectivity function

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Note: $\rho(A) \leq k + 1 \Leftrightarrow A$ is $k + 1$-separator $\Leftrightarrow A$ is k-module for P

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Create a hierarchical family $\texttt{Mod}$ of k-modules

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The hierarchic family $\mathtt{Mod}$ of subsets of $\mathcal{N}$ thus created has property: If $C \in \mathtt{Mod}$ then $\exists A, B \in \mathtt{Mod}$, $A \cap B = \emptyset$, $C = A \cup B$.

Vertex enumeration

For module $A \in \texttt{Mod}$ let

$$P^A := \{x \in \mathbb{R}^A : S_A x = D^A \alpha + d, x \geq 0, \exists \alpha \in \mathbb{R}^k\}.$$

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Definition (A-cface (combinatorial represent. of A-face))

For $A \subseteq \mathcal{N}$ a set $F \subseteq A$ is called a *A-cface* if there exists a $x \in P$ with $x_F = 0$ and $x_{A \setminus F} > 0$.

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Testing if $F \subset A$ is injective can be done in polytime

Injective cFase Enumeration

Recursively for every $C = A \dot{\cup} B$.
Let $\mathcal{F}^A :=$ Injective A-cFaces
Let $\mathcal{F}^B :=$ Injective B-cFaces

Construct

$$\mathcal{F} := \{F^A \cup F^B : F^A \in \mathcal{F}^A, F^B \in \mathcal{F}^B\}$$

For every $F \in \mathcal{F}$ test if it is a cface and injective for C.
If not delete F from $\mathcal{F}$

Set the resulting set $\mathcal{F}$ to $\mathcal{F}^C$

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The injective $\mathcal{N}$-cfaces are the vertices of P and Injective cFace Enumeration Algorithm applied to $C = \mathcal{N}$ computes all vertices of P.

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Did we not enumerate too many minimal faces on the way?

Vertex enumeration in total polytime

Proposition

Every injective and vertex inducing A-cface F for $A \in \texttt{Mod}$ *has* $\dim\{x \in P^A : x_F = 0\} \leq k$.

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For A-cface F, $A \in \texttt{Mod}$*, there exist* $\ell \leq k+1$ *vertex inducing A-cfaces* $F^1, \ldots, F^\ell$ *such that* $F = F^1 \cap F^2 \cap \ldots \cap F^\ell$.

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Proposition

If P is bounded then holds for all $A \in \texttt{Mod}$ that

$$|\{F \subseteq A : F \text{ injective } A\text{-cface}\}| \leq$$
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Let t time to test for injectiveness and the cface property.

Theorem

For P bounded and $A, B, C \in \texttt{Mod}$ with $C = A \dot{\cup} B$. Given the set of injective A-cfaces $\mathcal{F}^A$ and the set of injective B-cfaces $\mathcal{F}^B$, the set of injective C-cfaces $\mathcal{F}^C$ can be computed in time $O\left(|\mathcal{V}|^{2k+2} t\right)$,

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Since there are $O(\mathcal{N})$ internal nodes in the binary tree defining $\texttt{Mod}$, we have

Theorem

For P bounded its set of vertices can be computed in time $O\left(\mathcal{N}|\mathcal{V}|^{2k+2} t\right)$,

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  - Can the vertex with minimum size support of a k-modular polyhedron be found in polynomial time?