Cycles and Bicycles

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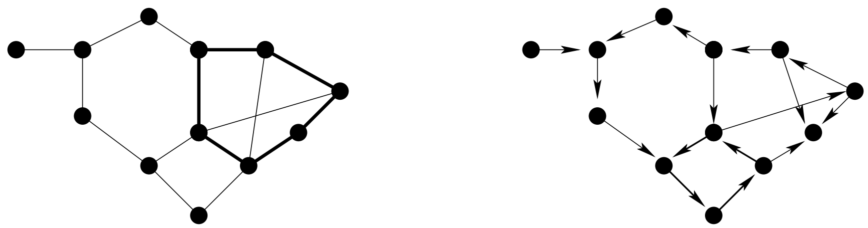
Undirected Graphs

We consider cycles in simple undirected or directed graphs $G(V, E)$.
$E \ldots$ edge set
$V \ldots$ vertex set



In the directed case we distinguish
cycles ... without orientation
circuits ... following the orientation of the edges.

$U \subseteq E \ldots |E|$-dimension vector (indexed by the edges):

A cycle (=subgraph with even vertex degrees) is an edge-disjoint union of *elementary cycles*.

TWO-CONNECTED GRAPHS only: every edge is contained in a cycle.

Vector Spaces of Edges

$$U_e = \begin{cases} 1 & \text{if} \quad e \in U \\ 0 & \text{if} \quad e \notin U \end{cases}$$

Incidence matrix $\mathbf{H}$ of G:

$$H_{xe} = \begin{cases} 1 & \text{if} \quad x \in e \\ 0 & \text{if} \quad x \notin e \end{cases}$$

All cycles satisfy

$$\mathbf{H}U = 0 \text{ over GF}(2) = (\{0,1\}, \oplus, \cdot)$$

Cycle space $\mathfrak{C}$ = vector space spanned by cycles

Dimension:

$$\dim \mathfrak{C} = \gamma(G) = |E| - |V| + \text{components}(G)$$

Bases of a Vector Space

A set $\{x_1, \ldots, x_L\}$ of vectors is *linearly independent* if the linear equation

$$\lambda_1 x_1 + \lambda_2 x_2 + \ldots \lambda_l x_l = 0$$

has no solution except $\lambda_1 = \lambda_2 = \cdots = \lambda_L = 0$.

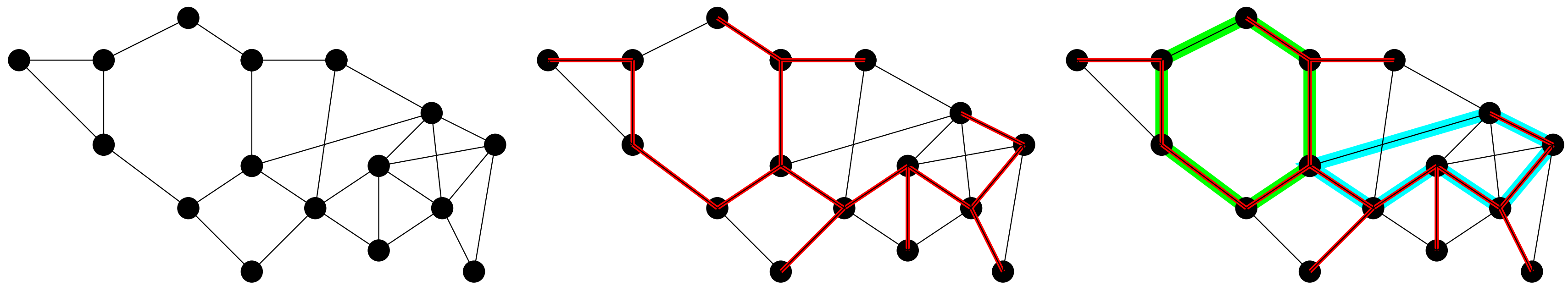
A basis of a vector space is a maximal set of linearly independent vectors.

Each vector x can be written as a linear combination of the basis elements $\mathcal{B} = \{y_1, y_2, \ldots, y_n\}$:

$$x = \lambda_1 y_1 + \lambda_2 y_2 + \cdots + \lambda_n y_n$$

Cycle Bases

Kirchhoff basis:



graph $\Rightarrow$ spanning tree $\Rightarrow$ cycles $C(T,e)$ for all $e \notin T$.

A basis of $\mathcal{B}$ is a Kirchhoff basis (or a *strictly fundamental* basis) of $\mathfrak{C}$ if there is a spanning tree T such that $\mathcal{B} = \{C(T,e) | e \in E \backslash T\}$.

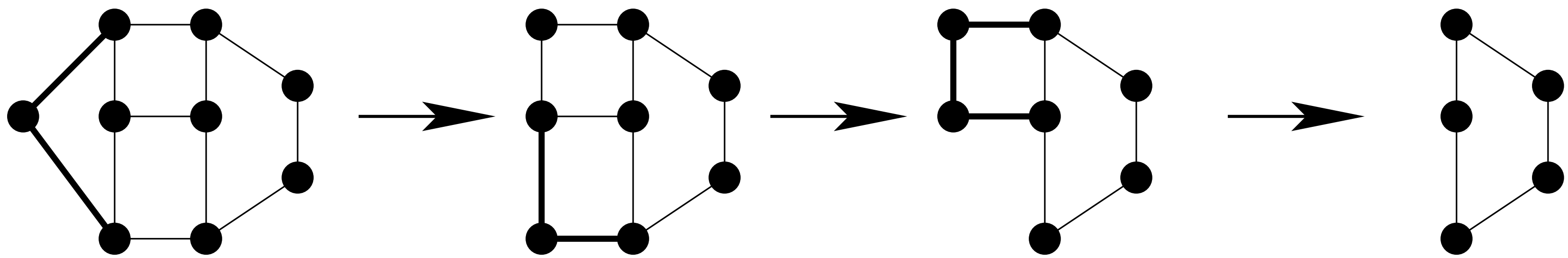
Fundamental Cycle Bases

A collection of $\nu(G)$ cycles in G is called *fundamental* if there is an ordering of these cycles such that

$$C_j \setminus (C_1 \cup C_2 \cup \cdots \cup C_{j-1}) \neq \emptyset \qquad \text{for } 2 \leq j \leq \nu(G)$$

Strictly Fundamental implies fundamental but not *vice versa*.

Ear Decomposition



Every two-connected graph has an ear decomposition. Each ear decomposition defines a basis of the cycle space $\mathfrak{C}$.

Minimal Length Cycle Bases

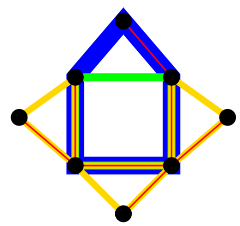
Length $|C|$ of cycle C = number of edges

Length of a cycle basis $\ell(\mathcal{B}) = \sum_{C \in \mathcal{B}} |C|$.

Relevant Cycles (Plotkin '71, Vismara '97);

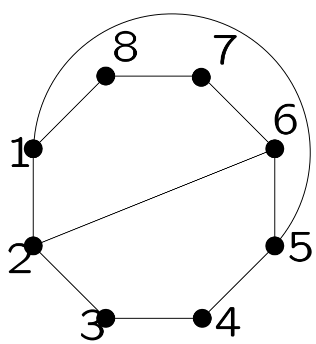
C is contained in a minimal cycle basis
$\Longleftrightarrow$
C cannot be written as a $\oplus$-sum of shorter cycles

Some Counter examples

- Not every MCB is strictly fundamental (Horton, Deo) 

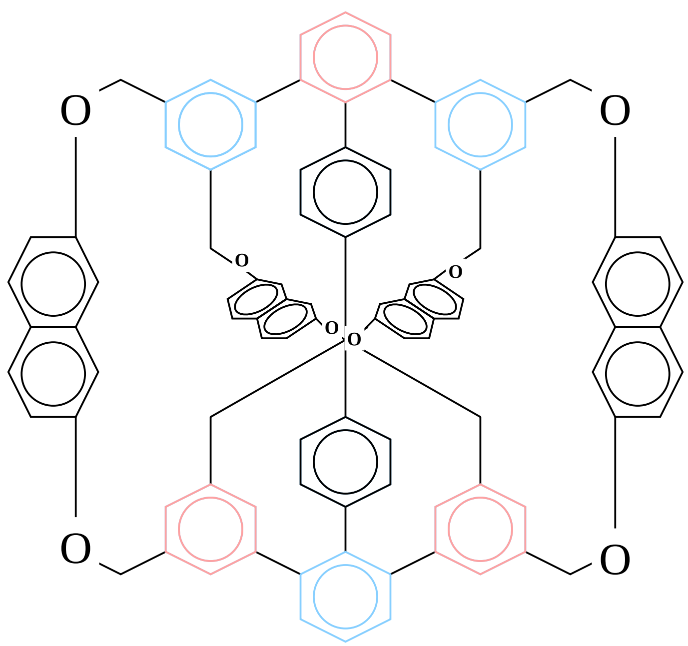
- Not every MCB is fundamental (examples are quite complicated)

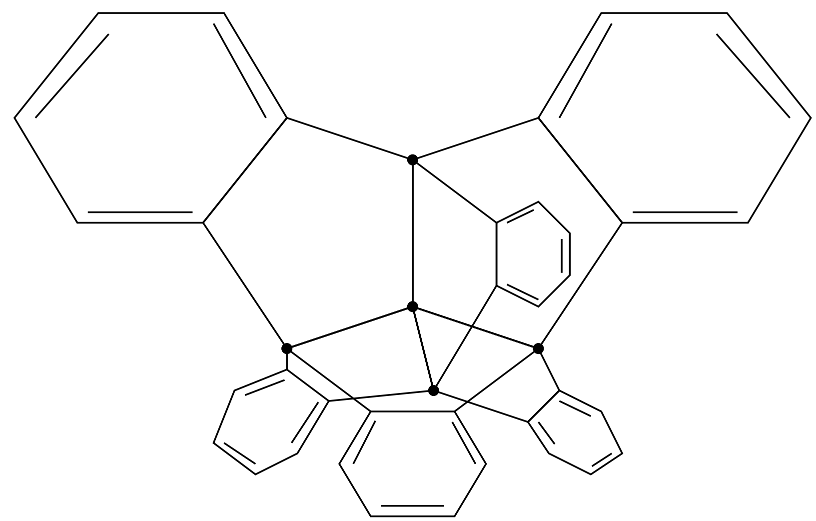
- The MCB of a planar graph not necessarily consists of faces



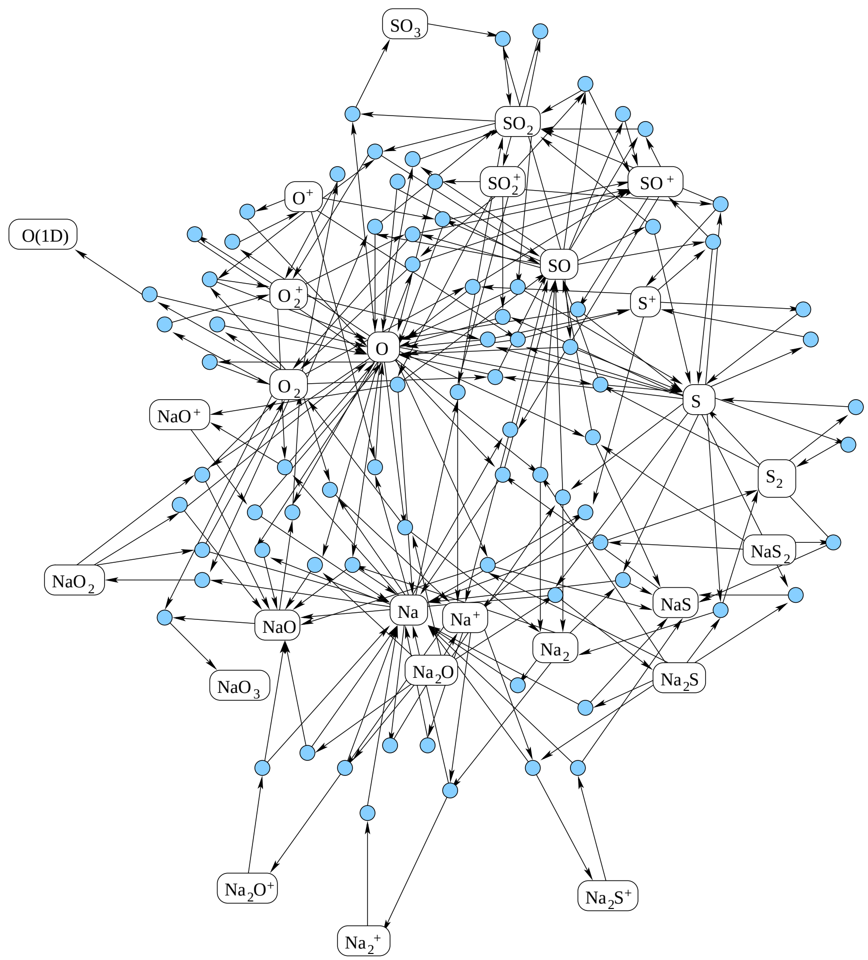
Who cares about MCBs?

Chemical Ring Perception (SSSR).





Analysis of chemical reaction networks.



Reaction network of Io's athmosphere

Matroid Property

The cycles of G form a matroid $\Longrightarrow$
A minimal cycle basis is obtained from the set of all cycles by a greedy procedure:

1. Sort set $\mathcal{C}$ of cycles by length

   $\mathcal{B} \leftarrow \emptyset$

2. while($\mathcal{C} \neq \emptyset$)

   $\mathcal{C} \leftarrow \mathcal{C} \setminus \{C\}$

   if $\mathcal{B} \cup \{C\}$ independent: $\mathcal{B} \leftarrow \mathcal{B} \cup \{C\}$.

Problem: exponentially many cycles.

Necessary conditions:

elementary (all vertices have degree 2)

short (isometric) for all vertices x, y in C, the cycle C contains a shortest paths between x and y.

Horton's Polynomial Time Algorithm

A cycle is *edge short* if C contains an edge $e = \{x, y\}$ and a vertex z such that

$$C = \{x, y\} \cup P(x, z) \cup P(y, z)$$

where $P(x, z)$ and $P(y, z)$ are shortest paths.

If C is relevant then it is edge-short
(Horton'87).

Construct (at most) $|E| \times |V|$ edge-short cycles.

Horton showed that even if $P(x, z)$ is not unique one may choose any shortest path, i.e., the $|E| \times |V|$ cycles contain a minimal cycle basis.

Alternative trick [Hartvigsen'94]: small perturbation of edge length to make minimum weight cycle basis unique.

Graph Operations

The length of minimal cycle bases does not behave "well" under many simple graph operations:

G_1 G_2

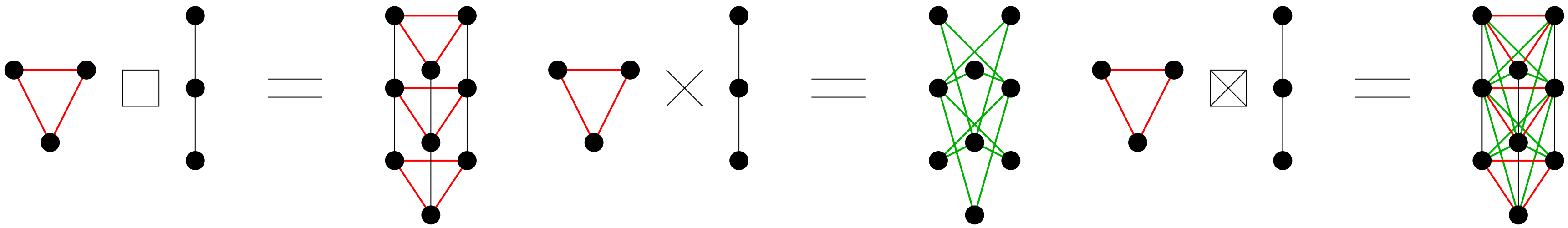
G_1 has $\nu(G_1) = 3$ and $\ell(G_1) = 38$. Deletion of a single edge leads to G_2 with $\nu(G_2) = 2$ but $\ell(G_2) = 44$.

Similar: other graph minor operations.

Cartesian and Strong Graph Products

Given two non-empty graphs $G = (V_G, E_G)$ and $H = (V_H, E_H)$:

Cartesian product $G \Box H$:
Vertex set $V_G \times V_H$
Edges: $(x_1, x_2)(y_1, y_2)$ is an edge in $E_{G \Box H}$ iff either $x_2 = y_2$ and $x_1 y_1 \in E_G$ or if $x_1 = y_1$ and $x_2 y_2 \in E_H$



Direct product $G \times H$:
Vertex set $V_G \times V_H$
Edges: $(x_1, x_2)(y_1, y_2)$ is an edge if $x_1 y_1 \in E_G$ and $x_2 y_2 \in E_H$

Strong product $G \boxtimes H$:

Vertex set $V_G \times V_H$

Edges: those of the direct product and those of the Cartesian product

Relevant Cycles in Product Graphs

$G = (V_G, E_G)$ and $H = (V_H, E_H)$ be two non-empty graphs,
T_G and T_H spanning trees,
$\mathcal{B}_G$ and $\mathcal{B}_H$ cycle bases of G and H.

Hammack's Basis for Cartesian Products (1999):

$$\mathcal{H}_1 = \{e\Box f | e \in T_G,\, f \in T_H\}$$
$$\mathcal{H}_2 = \{C^y | C \in \mathcal{B}_G,\, y \in V_H\}$$
$$\mathcal{H}_3 = \{{}^xC | x \in V_G,\, C \in \mathcal{B}_H\}$$
$$\mathcal{B}^* = \mathcal{H}_1 \cup \mathcal{H}_2 \cup \mathcal{H}_3$$

$\mathcal{B}^*$ is i general **not** minimal even if $\mathcal{B}_G$ and $\mathcal{B}_H$ are minimal.
- *Counterexample:* $C_5 \Box K_2$

Hammack basis: 4 squares and 2 pentagons.
Minimal length basis: 5 squares and 1 pentagon.

Hammack's basis is minimal if $\mathcal{B}_G$ and $\mathcal{B}_H$ consist of triangles and squares only.

Consider a triangle-free graph for the moment.

Idea. Start with the Hammack basis and replace as many cycles in the fibres as possible by squares from
$\mathcal{C}_\Box = \{e \Box f | e \in E_G, f \in E_H\}$.

Lemma. For all $C \in \mathcal{B}_G$ and all $x, y \in V_H$ there is a collection of squares in $\mathcal{C}_\Box$ such that
$C^x = C^y \oplus$ squares.

It is hence sufficient to have one copy $\mathcal{B}_G$ and one copy of $\mathcal{B}_H$ in one G and one H-fibre. The rest of the basis can be completed from $\mathcal{C}_\Box$.

To show that there are no relevant cycles that are not contained in $\mathcal{C}_\square$ or a fibre we consider the following procedure:

Set $\delta(x)$ = sum of distance of $x \in G\square H$ from two fixed fibres. Define for any cycle C^* in $\square H$:

$$\delta(C^*) = \sum_{x \in V_{C^*}} \frac{\mathrm{deg}_{C^*}(x)}{2} \delta(x),$$

We show that we keep adding squares from $\mathcal{C}_\square$ to C^* until we arrive at $\delta(C^{(k)}) = 0$ and $|C^{(k)}| \leq |C^*|$. Since C^* is either strictly shorter than C^* or it is the edge-disjoint union of a cycle in ${}^xH$ and a cycle in G^y C^* cannot be relevant.

It remains to show that it is impossible to replace any further basis cycle by squares from $\mathcal{C}_\square$. (not hard)

For graphs with triangles: retain triangles in each fibre and use the longer basis cycles in a single fibre only.

Total Basis Length in Iterated Products

$$\begin{aligned}\ell(G\Box H) = \ell(G) + \ell(H) + \\ 3\big[t_G(|V_H|-1) + 3t_H(|V_G|-1)\big] \\ + 4\big[(|E_G|-t_G)(|V_H|-1) + |E_H|-t_H)(|V_G|-1) - \\ (|V_H|-1)(|V_G|-1)\big]\end{aligned}$$

Substitute

$$G^n = G\Box G^{n-1} \simeq G^{n-1}\Box G, \qquad G^1 = G$$

and set $a = |E|/|V|$ and $\tau = t_G/|V|$, where t_G is the number of triangles in the MCB of G.

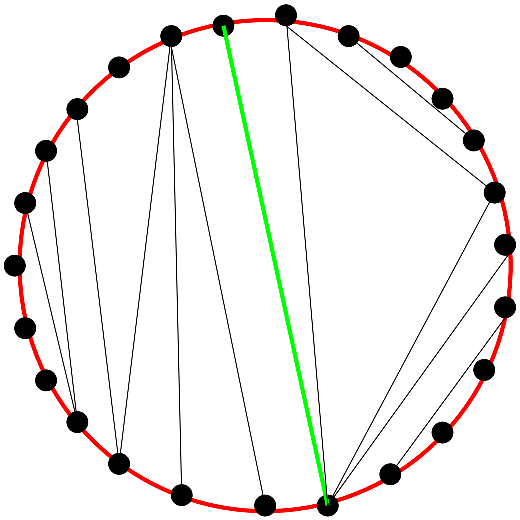
$$\begin{aligned}\ell(G^{n+1}) = \ell(G) + \ell(G^n) + 3\tau\big[|V|(|V^n|-1) + n|V|^n(|V|-1)\big] \\ + 4(a-\tau)\big[|V|(|V|^n-1) + n|V|^n(|V|-1) \\ - (|V|^n-1)(|V|-1)\big].\end{aligned}$$

Dividing by $\nu(G^{n+1})$ and setting $\xi = 1/V$ eventually yields:

$$L_\infty = \lim_{n\to\infty} L_n = 3\frac{\tau}{a} + 4\frac{a-\tau}{a}.$$

Graphs with a Unique MCB

Outerplanar graphs
Two-connected o.p. graphs have a Hamiltonian Cycle H and
each chord separates G into 2 two-connected outerplanar graphs G_1 and G_2.

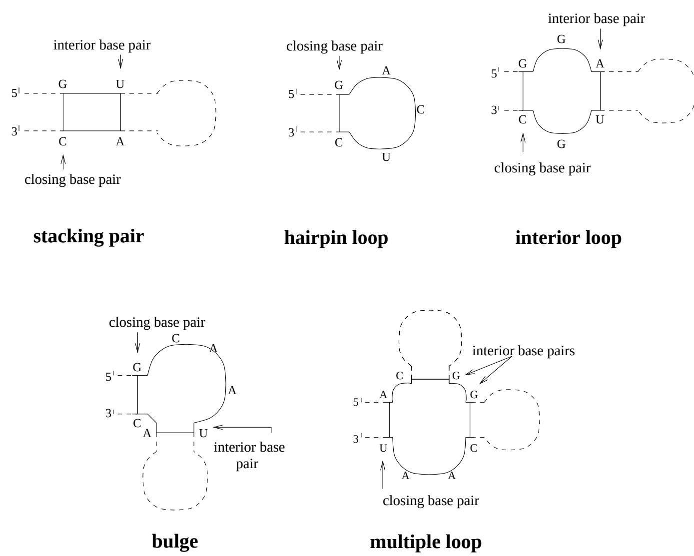


Take an edge e in H. The shortest cycle C through e contains at least one chord, hence C is a member of the MCB. Split C along the chords and repeat.

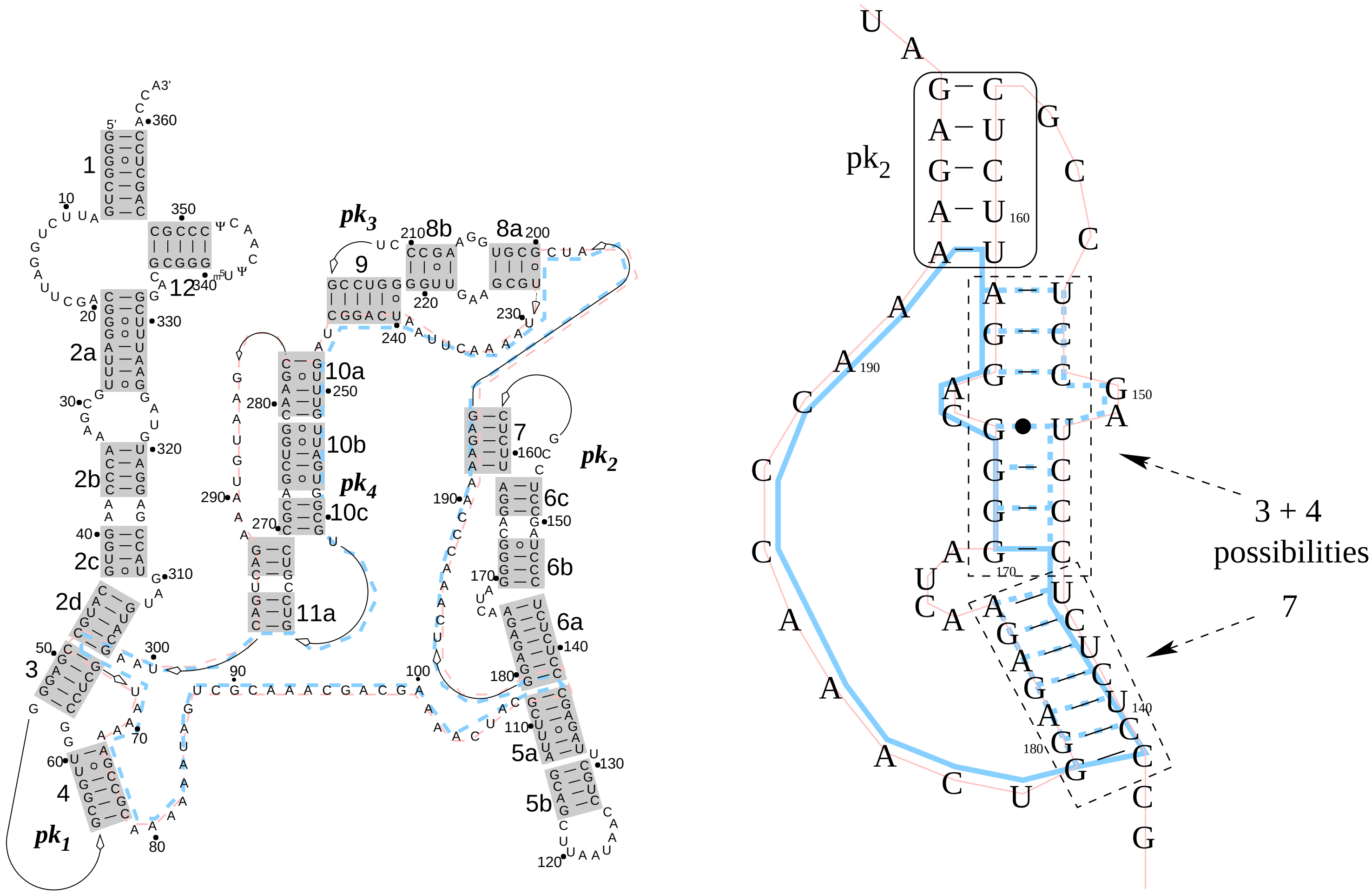
RNA Secondary Structures

outerplanar.

"loops" = cycles of the **unique** MCB.



Pseudoknots: MCB usually not unique.



tmRNA from E.coli with its pseudoknots

Exchangability of Relevant Cycles

Set $\mathcal{R}$ of relevant cycles of an undirected graph can be computed efficiently by Vismara's algortithm (1997).

Def.: $C, C' \in \mathcal{R}$ are exchangable, $C \leftrightarrow C'$, if there is a set $\mathcal{Q}$ of relevant cycles such that
(i) $|C''| \leq |C| = |C'|$ for all $C'' \in \mathcal{Q}$,
(ii) $\mathcal{Q} \cup \{C'\}$ is linearly independent, and
(iii) $C' = C \cup \bigoplus \mathcal{Q}$.

Theorem. $C \leftrightarrow C'$ is an equivalence relation.

Surprisingly tedious to prove ...

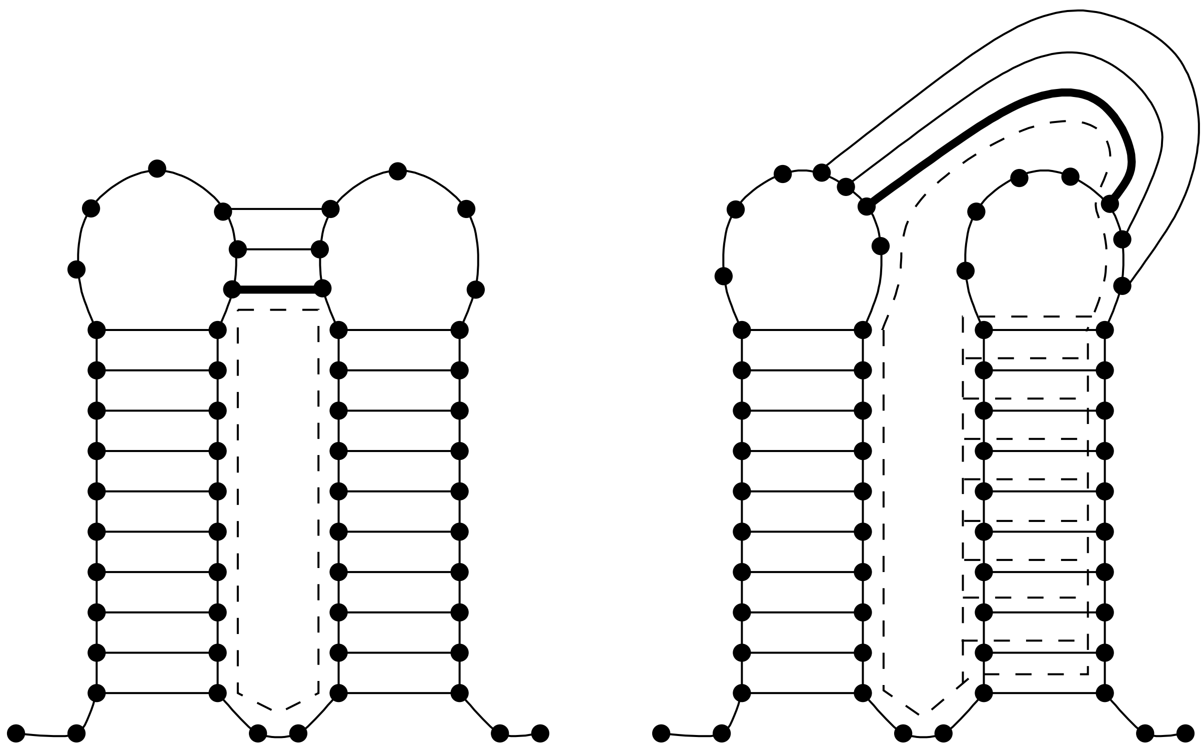
uses explicitly that we work over GF(2), i.e.,

does not work for general matroids.

Theorem. Let $\mathcal{W}$ be a $\leftrightarrow$-class and let $\mathcal{M}$ be a minimal cycle basis. Then

$$\mathrm{knar}(\mathcal{W}) = |\mathcal{M} \cap \mathcal{W}|$$

is independent of the choice of the minimal cycle basis $\mathcal{M}$.



Directed Graphs

Let $G(V, A)$ be a directed graph and a U a cycle in G.
Associated vector:

$$U_e = \begin{cases} +1 & \text{if} \quad e \in U \quad \text{in forward direction} \\ -1 & \text{if} \quad e \in U \quad \text{in backward direction} \\ 0 & \text{if} \quad e \notin U \end{cases}$$

Incidence matrix $\mathbf{H}$ of G:

$$H_{xe} = \begin{cases} -1 & \text{if} \quad x \text{ is inital point of arc } e \\ +1 & \text{if} \quad x \text{ is terminal point of arc } e \\ 0 & \text{if} \quad x \notin e \end{cases}$$

All cycles satisfy

$$\mathbf{H}U = 0 \text{ over } \mathbb{R}$$

Circuit cycle in forward direction, $C_e = 0, +1$.

Circuit Bases

Theorem. (Berge) If $G(V, A)$ is strongly connected if it has a cycle basis consisting of (elementary) circuits.

Remark. Elementary circuits generate the extremal rays of the convex cone

$$\mathbb{K} := \{U : \mathbf{H}U = 0 \quad \text{and} \quad U(e) \geq 0\}$$

How to compute a minimum length circuit basis?

Circuits again form a matroid (linear independence over $\mathbb{R}$).

$\Longrightarrow$ Greedy Algorithm.

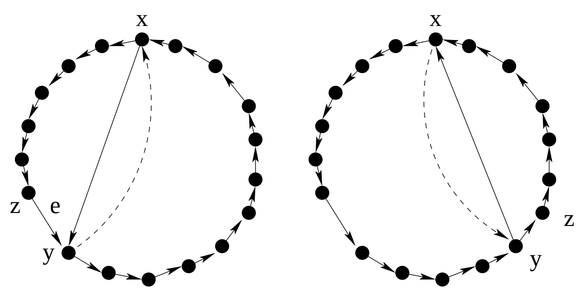
Again exponentially many circuits.

Def. A circuit C is *short* if for all vertices x and y it contains a shortest path $S[x, y]$ *or* a shortest path $S[y, x]$.

Def.: A circuit C is *arc-short* if C contains a vertex x and an arc $e = (v, w)$ such that $C = P[w, x] + P[x, v] + (v, w)$ where $P[w, x]$ and $P[x, v]$ are shortest directed paths.

Lemma. If C is short, it is arc-short

Proof.



Lemma. If C is relevant, then C is short.

Proof. C relevant but not short $\Longrightarrow$
$\exists x, y$ in C: C contains neither shortest paths $S[x, y]$ nor $S[y, x]$. Then $C^1 = C[x, y] + S[y, x]$, $C^2 = S[x, y] + S[y, x]$, and $C^3 = S[x, y] + S[y, x]$ are closed paths in G and hence are sums of (shorter) circuits. Furtermore

$$C = C[x, y] + C[y, x] = C^1 + C^2 - C^3$$

and $|C^i| < |C|$

Minimum Circuit Base

1: Compute directed distances and shortest paths with perturbed edge length. $\mathcal{O}(|V|^3)$

2: Construct $|A| \times |V|$ candidates for arc-short cycles.

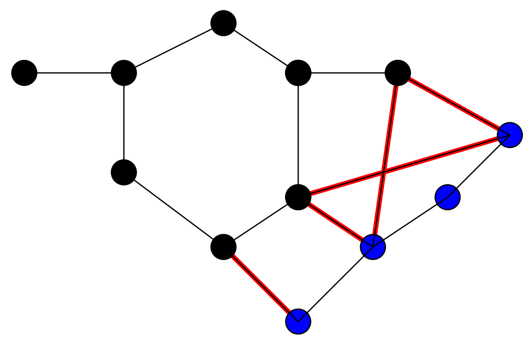
3: Check that the cycles are elementary. $\mathcal{O}(|V|)$ for each cycle, i.e., $\mathcal{O}(|A| \times |V|^2)$

4: Greedy step. At most $|A| \times |V|$ Gauss eliminations on a $(\nu(G) + 1) \times |E|$ matrix, i.e., at most $\mathcal{O}(\nu(G)|E|^2 \times |V|)$.

For most graphs probably much faster.

Cuts

Let (V_1, V_2) be a partition of the vertex set V, i.e., $V_1, V_2 \neq \emptyset$ and $V_1 \cup V_2 = V$.



A **cut** or **cocycle** $K = \langle V_1, V_2 \rangle$ is the set of all edges in G that have one end in V_1 and one end in V_2.

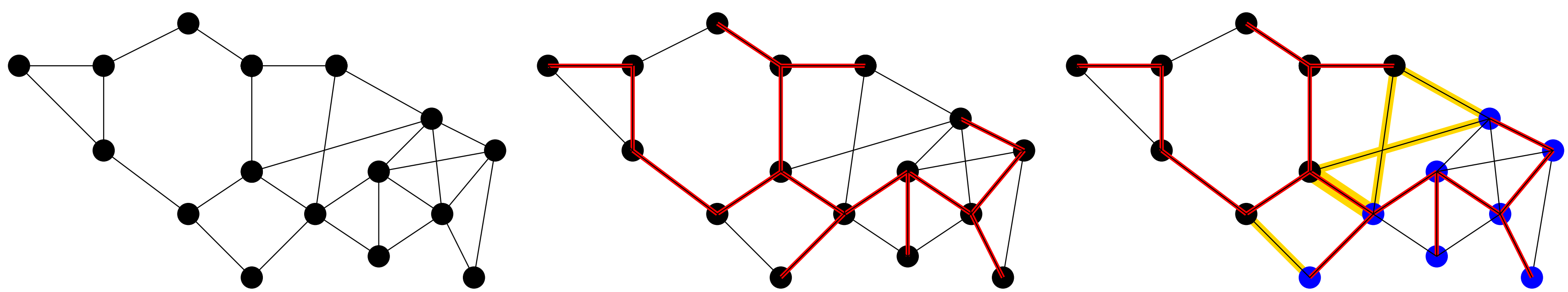
The cuts form a vector space $\mathfrak{K}$ over $(\{0,1\}, \oplus, \cdot)$ with dimension $|V| - 1$.

Fundamental Cuts

A basis is again obtained from a spanning tree: Let $b \in T$. Removal of b disconnects the tree T into exactly two subtrees with vertex sets $V_1^{T,b}$ and $V_2^{T,b}$. The cut

$$\text{cut}(T,b) := \langle V_1^{T,b}, V_2^{T,b} \rangle$$

is *fundamental cut* of G.



T has $|V|-1$ edges, thus there are $|V|-1$ linearly independent fundamental cuts.

Cut Sets

A cut is a *cut set of* G if both V_1 and V_2 are connected.

$\Rightarrow$ every fundamental cut cut(T, b) is a cut set of G. ($T \setminus \{b\}$ consists of two trees)

Size of a cut: $|K|$

Length of a cut basis $\ell(\mathcal{B}) = \sum_{K \in \mathcal{B}} |K|$

Minimal basis of the cut space?

The Cut Tree

Let $G(V, E)$ be a graph, possibly with edge weights $w(e)$.

A *cut tree* $T^{\#}$ of G is a tree with vertex set V with the following property:
For every pair of distinct vertices $s, t \in V$, let e be a minimum weight edge on the unique path from s to t in $T^{\#}$. Deleting e from $T^{\#}$ separates $T^{\#}$ into two connected components $V_1^{st,e}$ and $V_2^{st,e}$ such that

$$\text{cut}(T^{\#}; e) = \langle V_1^{st,e}, V_2^{st,e} \rangle$$

is a minimum weight cut separating s, t.

The algorithms by Gomory and Hu (1961) and Gusfield (1991) compute a cut tree $T^{\#}$ and the sets cut$(T^{\#}; e)$ in $\mathcal{O}(|E||V|^2 \log |V|)$ steps.

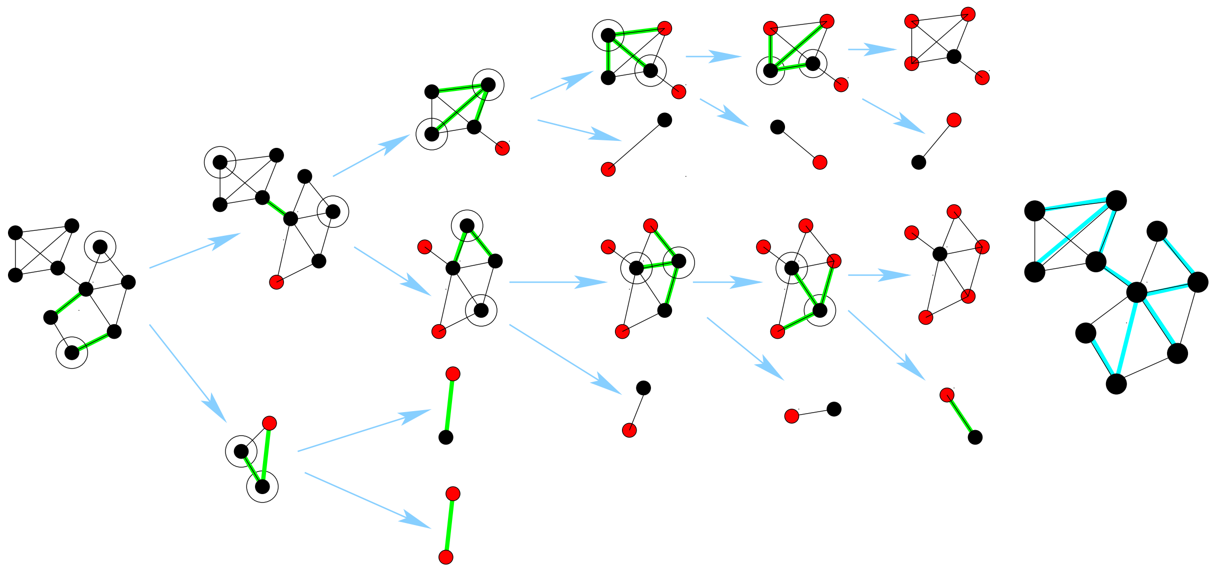
The Gomory-Hu Algorithm

In a nutshell:

(1) Pick two vertices s and t (at random) and find the minimum weight cut (V_1, V_2) that separates s and t.

(2) Form two graphs G_1 and G_2 by contracting V_2 and V_1, repectively.

(3) Repeat with both graphs until only graphs with two vertices as left.



Lemma. (see e.g. Golynski, Horton 2001)
If $T^{\#}$ is a cut tree then

$$\mathcal{M} = \{\text{cut}(T^{\#}; e) | e \in T^{\#}\}$$

is a minimum weight basis of the cut space $\mathfrak{K}$.

Proof. We use the edge-weight perturbation trick to make the Gomory-Hu tree and all cut weights unique.

Suppose $\mathcal{Q}$ is a minimal cut basis and let $H = \text{cut}(T^{\#}; e)$ be the minimum weight cut separating s and t. Then H is a $\oplus$-sum of cuts in $\mathcal{Q}$. This sum must contain a cut H' which separates s and t. Suppose $H \neq H'$. Of course, H' cannot be shorter than the cut H, hence $\mathcal{Q}' = \mathcal{Q} \setminus \{H'\} \cup \{H\}$ is shorter than $\mathcal{Q}$, a contradiction to minimality. Thus $\text{cut}(T^{\#}; e) \in \mathcal{Q}$. This holds for each of the $|V| - 1$ cuts associated with $T^{\#}$, which are linearly independent, and the lemma follows from $\dim \mathfrak{K} = |V| - 1$.

Open Question: How to compute the set of relevant cuts in the unweighted (or degenerate) case?

Relationships of Cycles and Cuts

$C \in \mathfrak{C}$ if $|C \cap K|$ is even for *all* $K \in \mathfrak{K}$.

$K \in \mathfrak{K}$ if $|C \cap K|$ is even for *all* $C \in \mathfrak{C}$.

Thus, for all $C \in \mathfrak{C}$ and all $K \in \mathfrak{K}$ $|C \cap K|$ is even, i.e.,

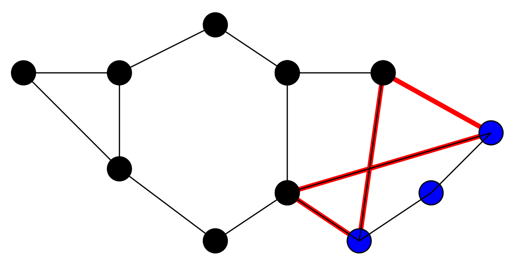
$$\bigoplus_{e \in E} C_e \cdot K_e = 0\,.$$

In other words $\mathfrak{C}$ and $\mathfrak{K}$ are "orthogonal" **over GF(2)**.

$\mathfrak{C}$ and $\mathfrak{K}$ are *orthogonal complements* iff $\mathfrak{C} \cap \mathfrak{K} = \{\emptyset\}$.

So what is a "bicycle"?

Def. A *bicycle* B is a subset of E that is both a cycle and a cocycle (cut).



Thus the *bicycle space* is $\mathfrak{B} = \mathfrak{C} \cap \mathfrak{K}$.

Some graphs have bicycles, some don't . . .

QUESTION: How can we compute (minimal) Bicycle Bases ???

Thanx!

Joint work with

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