Polyhedra

- *Hyperplane* $H = \{x \in \mathbb{R}^n \mid a^T x = \beta\}$, $a \in \mathbb{R}^n \setminus \{0\}, \beta \in \mathbb{R}$
- *Closed halfspace* $\overline{H} = \{x \in \mathbb{R}^n \mid a^T x \leq \beta\}$
- *Polyhedron* $P = \{x \in \mathbb{R}^n \mid Ax \leq b\}, A \in \mathbb{R}^{m \times n}, b \in \mathbb{R}^m$
- *Polytope* $P = \{x \in \mathbb{R}^n \mid Ax \leq b,\ l \leq x \leq u\}, l, u \in \mathbb{R}^n$
- *Polyhedral cone* $P = \{x \in \mathbb{R}^n \mid Ax \leq 0\}$

The feasible set

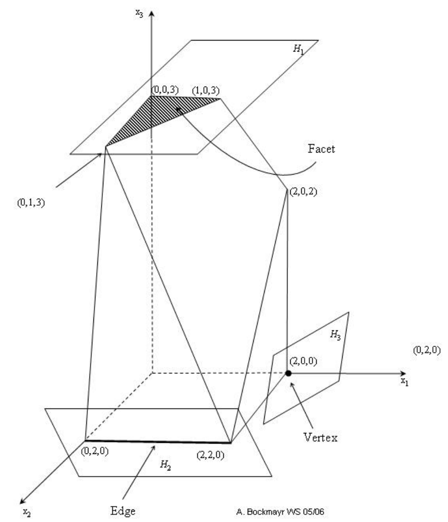
$$P = \{x \in \mathbb{R}^n \mid Ax \leq b\}$$

of a linear optimization problem is a polyhedron.

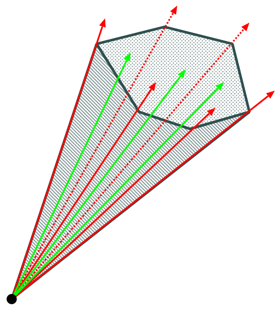
Vertices, Faces, Facets

- $P \subseteq \overline{H}, H \cap P \neq \emptyset$ *(Supporting hyperplane)*
- $F = P \cap H$ *(Face)*
- $\dim(F) = 0$ *(Vertex)*
- $\dim(F) = 1$ *(Edge)*
- $\dim(F) = \dim(P) - 1$ *(Facet)*
- *P pointed: P* has at least one vertex.

Illustration



Rays and extreme rays



- $r \in \mathbb{R}^n$ is a *ray* of the polyhedron P if for each $x \in P$ the set $\{x + \lambda r \mid \lambda \geq 0\}$ is contained in P.
- A ray r of P is *extreme* if there do not exist two linearly independent rays r^1, r^2 of P such that $r = \frac{1}{2}(r^1 + r^2)$.

Hull operations

- $x \in \mathbb{R}^n$ is a *linear combination* of $x^1, \ldots, x^k \in \mathbb{R}^n$ if

$$x = \lambda_1 x^1 + \cdots + \lambda_k x^k, \text{ for some } \lambda_1, \ldots, \lambda_k \in \mathbb{R}.$$

- If, in addition

$$\left\{ \begin{array}{ll} \lambda_1, \ldots, \lambda_k \geq 0, & \\ & \lambda_1 + \cdots + \lambda_k = 1, \\ \lambda_1, \ldots, \lambda_k \geq 0, & \lambda_1 + \cdots + \lambda_k = 1, \end{array} \right\} x \text{ is a } \left\{ \begin{array}{c} \textit{conic} \\ \textit{affine} \\ \textit{convex} \end{array} \right\} \text{combination.}$$

- For $S \subseteq \mathbb{R}^n, S \neq \emptyset$, the set $\text{lin}(S)$ (resp. $\text{cone}(S), \text{aff}(S), \text{conv}(S)$) of all linear (resp. conic, affine, convex) combinations of finitely many vectors of S is called the *linear (resp. conic, affine, convex) hull of* S.

Outer and inner descriptions

- A subset $P \subseteq \mathbb{R}^n$ is a *H-polytope,* i.e., a *bounded* set of the form *Outer*

$$P = \{x \in \mathbb{R}^n \mid Ax \leq b\}, \text{ for some } A \in \mathbb{R}^{m \times n}, b \in \mathbb{R}^m.$$

  if and only if it is a *V-polytope,* i.e., *Inner*

$$P = \text{conv}(V), \text{ for some finite } V \subset \mathbb{R}^n$$

- A subset $C \subseteq \mathbb{R}^n$ is a *H-cone,* i.e., *Outer*

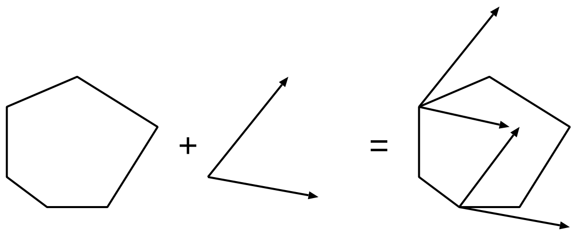
$$C = \{x \in \mathbb{R}^n \mid Ax \leq 0\}, \text{ for some } A \in \mathbb{R}^{m \times n}.$$

  if and only if it is a *V-cone,* i.e., *Inner*

$$C = \text{cone}(Y), \text{ for some finite } Y \subset \mathbb{R}^n$$

Minkowski sum

- $X, Y \subseteq \mathbb{R}^n$
- $X + Y = \{x + y \mid x \in X, y \in Y\}$ *(Minkowski sum)*



Main theorem for polyhedra

A subset $P \subseteq \mathbb{R}^n$ is a *H-polyhedron,* i.e., *Outer*

$$P = \{x \in \mathbb{R}^n \mid Ax \leq b\}, \text{ for some } A \in \mathbb{R}^{m \times n}, b \in \mathbb{R}^m.$$

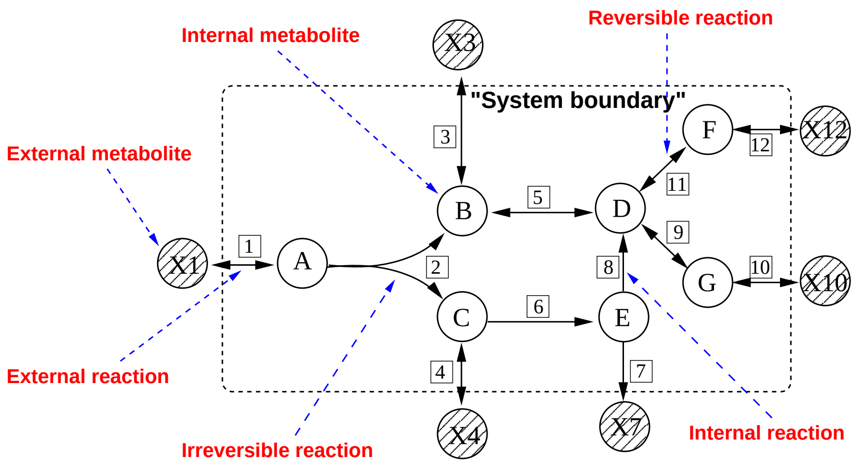
if and only if it is a *V-polyhedron,* i.e., *Inner*

$$P = \text{conv}(V) + \text{cone}(Y), \text{ for some finite } V, Y \subset \mathbb{R}^n$$

Theorem of Minkowski

- For each polyhedron $P \subseteq \mathbb{R}^n$ there exist finitely many points $p^1, \dots, p^k$ in P and finitely many rays $r^1, \dots, r^l$ of P such that
$$P = \text{conv}(p^1, \dots, p^k) + \text{cone}(r^1, \dots, r^l).$$
- If the polyhedron P is pointed, then $p^1, \dots, p^k$ may be chosen as the uniquely determined vertices of P, and $r^1, \dots, r^l$ as representatives of the up to scalar multiplication uniquely determined extreme rays of P.
- *Special cases*
  - A polytope is the convex hull of its vertices.
  - A pointed polyhedral cone is the conic hull of its extreme rays.

Application: Metabolic networks



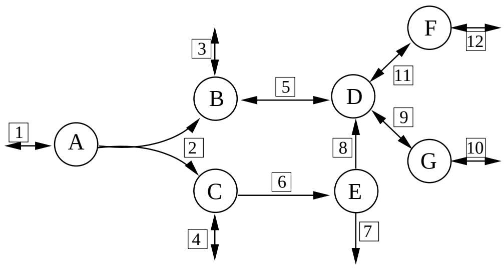
Stoichiometric matrix

- Metabolites (internal) $\rightsquigarrow$ rows

- Biochemical reactions $\rightsquigarrow$ columns

$$kA + lC \xrightarrow{j} mE + nH \qquad \begin{array}{c} A \\ B \\ C \\ D \\ E \\ F \\ G \\ H \end{array} \begin{pmatrix} \dots & -k & \dots \\ & 0 & \\ & -l & \\ & 0 & \\ & m & \\ & 0 & \\ & 0 & \\ \dots & n & \dots \end{pmatrix}$$

Example network



$$S = \begin{pmatrix} 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & -1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 \end{pmatrix}.$$

Flux cone

- Flux balance: $Sv = 0$
- Irreversibiliy of some reactions: $v_i \geq 0, i \in Irr$.
- *Steady-state flux cone*

$$C = \{v \in \mathbb{R}^n \mid Sv = 0, v_i \geq 0, \text{ for } i \in Irr\}$$

- *Metabolic network analysis* $\rightsquigarrow$ find $p^1, \dots, p^k \in C$ with $C = \text{cone}\{p^1, \dots, p^k\}$.