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**

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

**Illustration**
* $r \in \mathbb{R}^n$ 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

\[
\begin{align*}
\lambda_1, \ldots, \lambda_k &\geq 0, \\
\lambda_1 + \cdots + \lambda_k &\leq 1,
\end{align*}
\]

$x$ is a conic affine convex 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

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

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

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

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

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

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

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

### 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.,

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

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

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

Theorem of Minkowski

- For each polyhedron $P \subseteq \mathbb{R}^n$ there exist finitely many points $p_1, ..., p_k$ in $P$ and finitely many rays $r_1, ..., r_l$ of $P$ such that

  $$P = \text{conv}(p_1, ..., p_k) + \text{cone}(r_1, ..., r_l).$$

- If the polyhedron $P$ is pointed, then $p_1, ..., p_k$ may be chosen as the uniquely determined vertices of $P$, and $r_1, ..., r_l$ 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

\[
\begin{bmatrix}
A & ... & -k & ... \\
B & 0 & & \\
C & -l & 0 & \\
D & m & 0 & \\
E & 0 & 0 & \\
F & 0 & 0 & \\
G & 0 & 0 & \\
H & ... & n & ...
\end{bmatrix}
\]

Reaction \( kA + lC \xrightarrow{r} mE + nH \) gives

Flux cone

- Flux balance: \( \mathbf{Sv} = 0 \)
- Irreversibility of some reactions: \( v_i \geq 0, i \in \text{Irr.} \)
- Steady-state flux cone

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

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

Flux balance analysis

- Use linear programming to study flux distribution in a cell

\[
\max \{ \mathbf{c}^T \mathbf{v} \mid \mathbf{Sv} = 0, \ \mathbf{v}_{\min} \leq \mathbf{v} \leq \mathbf{v}_{\max} \}
\]

- Objective function
  - Maximize biomass production
  - Maximize metabolite production (e.g. biofuel)

- Metabolic engineering