The Geology of Gale Diagrams

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JAVA applet and Peterson's Masters thesis available at

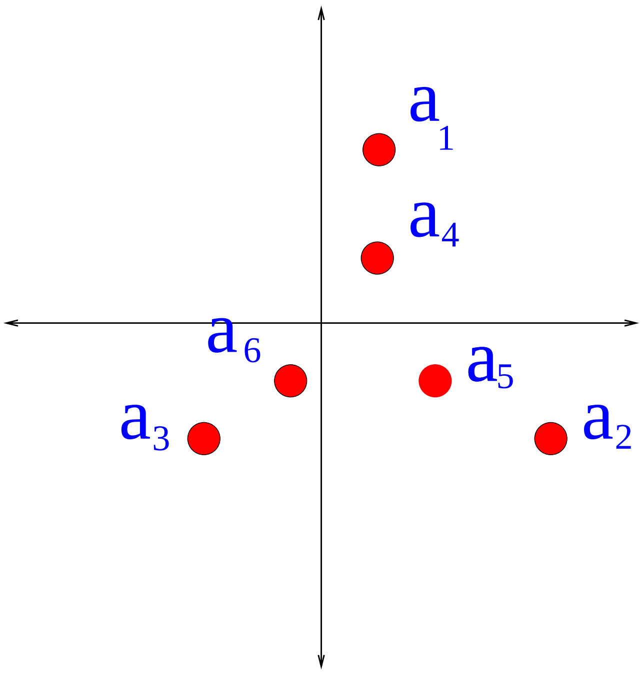
`www.math.umn.edu/~reiner/CHEMOGALE.html`

Outline:

I. Geometry (discrete)

II. Geology

$\mathcal{A} = \{a_1, \ldots, a_n\}$ is a finite collection of n points in $(d-1)$-dimensional space $\mathbb{R}^{d-1}$.

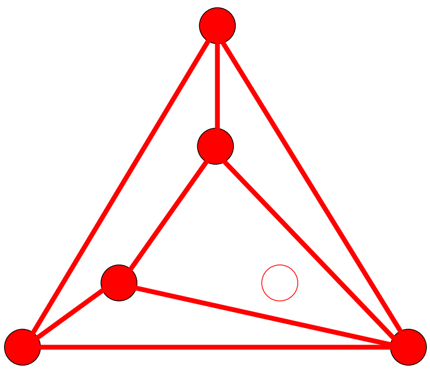


Here $\mathcal{A}$ has $n = 6$ and $d = 3$.

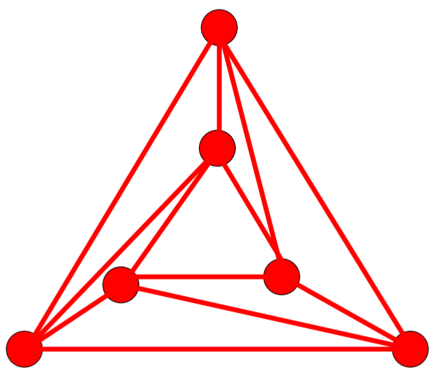
A triangulation Δ of $\mathcal{A}$ is a collection of simplices,

- covering the convex hull of $\mathcal{A}$
- using only vertices from the set $\mathcal{A}$ (but not necessarily using all of them)
- with every pair of simplices meeting along a common face (possibly empty) of each.

Two examples for the previous $\mathcal{A}$:



$\triangle_1$



$\triangle_2$

Say that a triangulation Δ of $\mathcal{A}$ is coherent if it arises from the following geometric construction:

(1) Choose a vector $g = (g_1, \ldots, g_n)$ of heights with which to lift each a_i in $\mathcal{A}$ from $\mathbb{R}^{d-1}$ to the point (a_i, g_i) in $\mathbb{R}^d$.

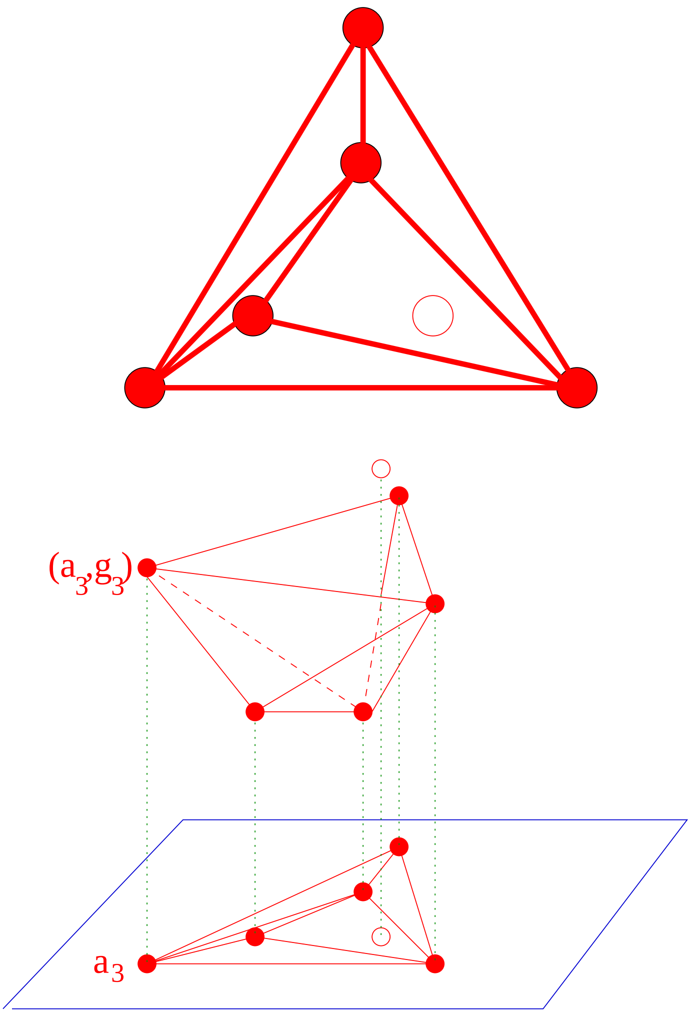
(2) Find the faces in the lower convex hull of these lifted points,

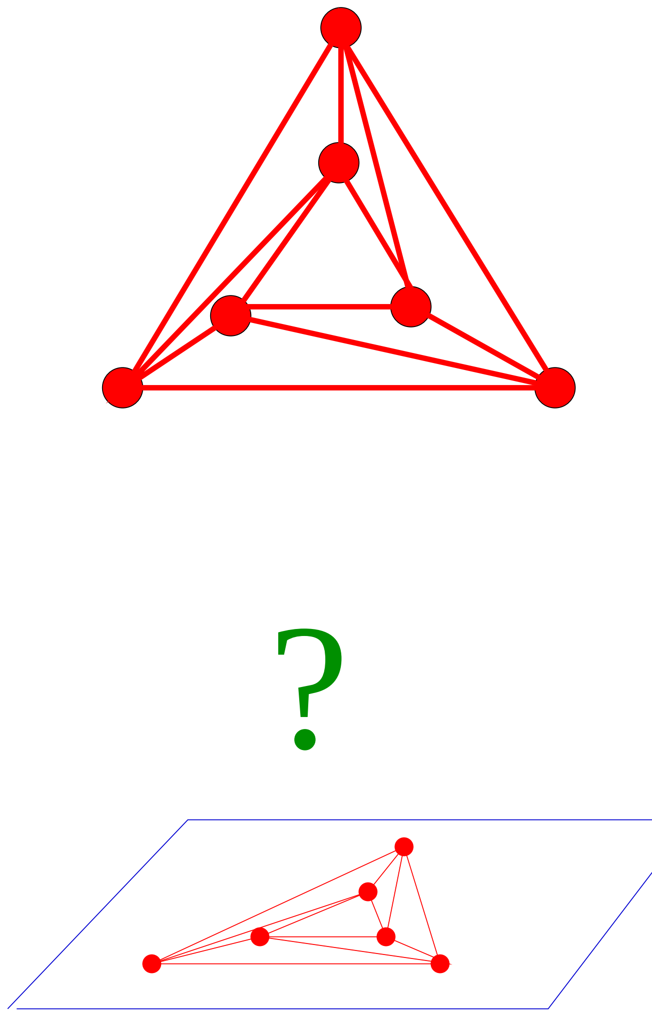
(3) Project these faces from $\mathbb{R}^d$ down to $\mathbb{R}^{d-1}$.

Denote by $\Delta(g)$ the coherent triangulation induced by the vector of heights $g = (g_1, \ldots, g_n)$ in $\mathbb{R}^n$.

Coherent

Incoherent





All triangulations of $\mathcal{A}$ are coherent

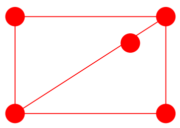
- when $d \leq 2$ (easy),
- when $n - d \leq 2$ (C. Lee 1991).

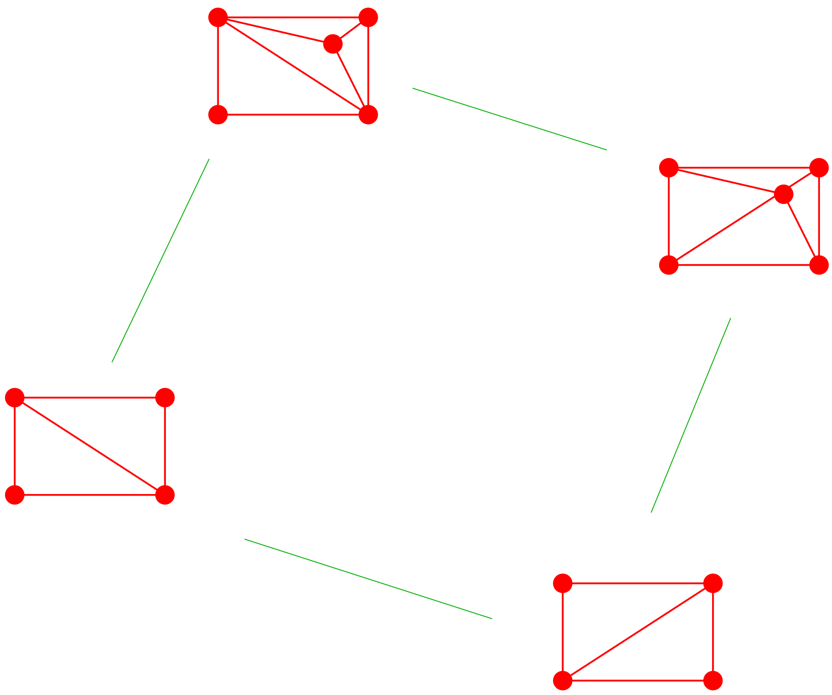
Under the hypotheses assumed by the geologists, only the *coherent* triangulations should arise in their applications.

Nevertheless, existence of incoherent triangulations is important for the geologists to be aware of, as this would warn that one of their *hypotheses must fail* to hold. Apparently incoherent triangulations were not widely known to them, if at all.

Is there structure on the set of all triangulations, or all coherent triangulations?

They are connected by local moves/modifications called bistellar operations.

$A=$ 



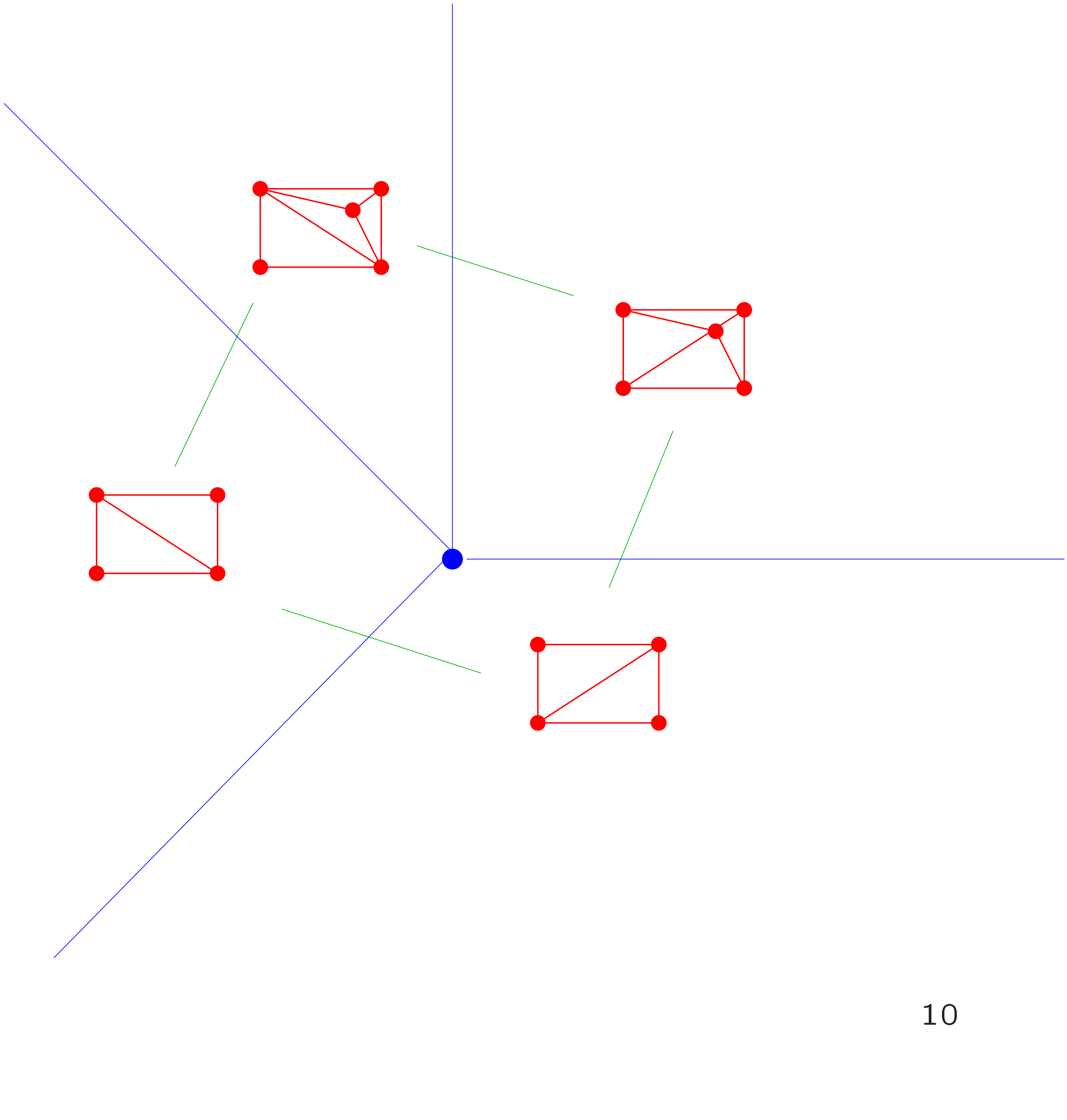
Why expect any such structure?
A related question: "When do two lifting vectors g, g' in $\mathbb{R}^n$ give rise to the same triangulations $\Delta(g) = \Delta(g')$?"

Equivalence classes on $\mathbb{R}^n$ ought to be polyhedral cones, fitting together into a complete fan that covers $\mathbb{R}^n$; this is called the secondary fan $\mathcal{F}(\mathcal{A})$.

n-dimensional cones of $\mathcal{F}(\mathcal{A})$ $\leftrightarrow$
coherent triangulations of $\mathcal{A}$

walls between these cones $\leftrightarrow$
bistellar operations

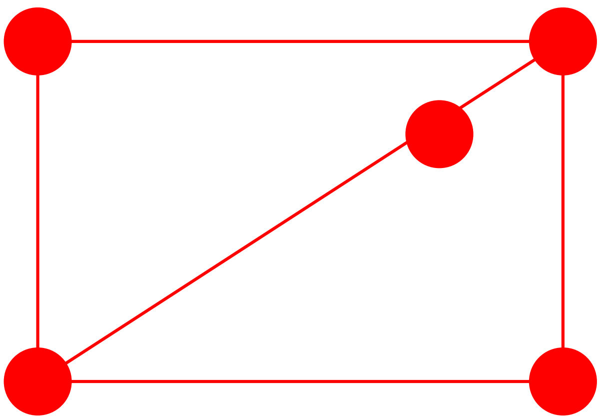
For example, with $\mathcal{A}$ as before, one can compute that $\mathcal{F}(\mathcal{A})$ looks like $\mathbb{R}^3 \times \mathcal{F}'(\mathcal{A})$, where $\mathcal{F}'(\mathcal{A})$ is the pointed secondary fan in $\mathbb{R}^2$ shown in blue below.



There is a simple recipe for finding $\mathcal{F}(\mathcal{A})$, $\mathcal{F}'(\mathcal{A})$, involving the Gale transform of $\mathcal{A}$.

Encode $\mathcal{A}$ as an $\mathsf{d} \times \mathsf{n}$ matrix A having column vectors $(a_i, 1)$ for each a_i in $\mathcal{A}$.

e.g. with $\mathcal{A}$ as before



we might have

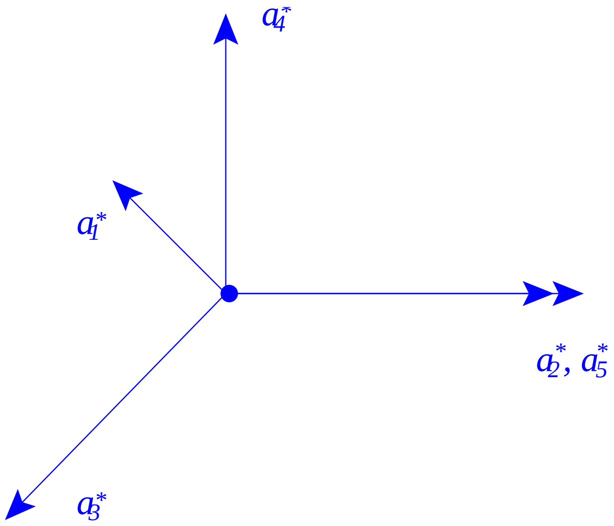
$$A = \begin{bmatrix} 0 & 3 & 2 & 3 & 0 \\ 0 & 0 & 2 & 3 & 3 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix}$$

Compute any $n-d \times n$ matrix A^* whose rows form a basis for the nullspace $\ker(A)$.

e.g.

$$A^* = \begin{bmatrix} -1 & 2 & -3 & 0 & 2 \\ 1 & 0 & -3 & 2 & 0 \end{bmatrix}$$

The columns $\mathcal{A}^* = \{a_1^*, \ldots, a_n^*\}$ are called a Gale transform of $\mathcal{A} = \{a_1^*, \ldots, a_n^*\}$.

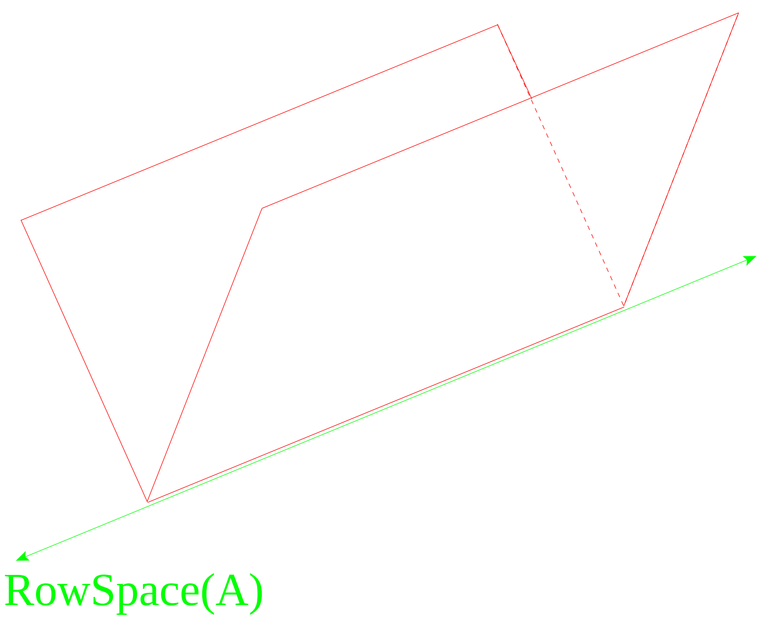


(Note it is "a" Gale transform because it is well-defined only up to the action of $GL(\mathbb{R}^{n-d})$.)

PROPOSITION If g, g' in $\mathbb{R}^n$ differ by an element in the row space of A , then they induce the same coherent triangulation $\Delta(g) = \Delta(g')$.

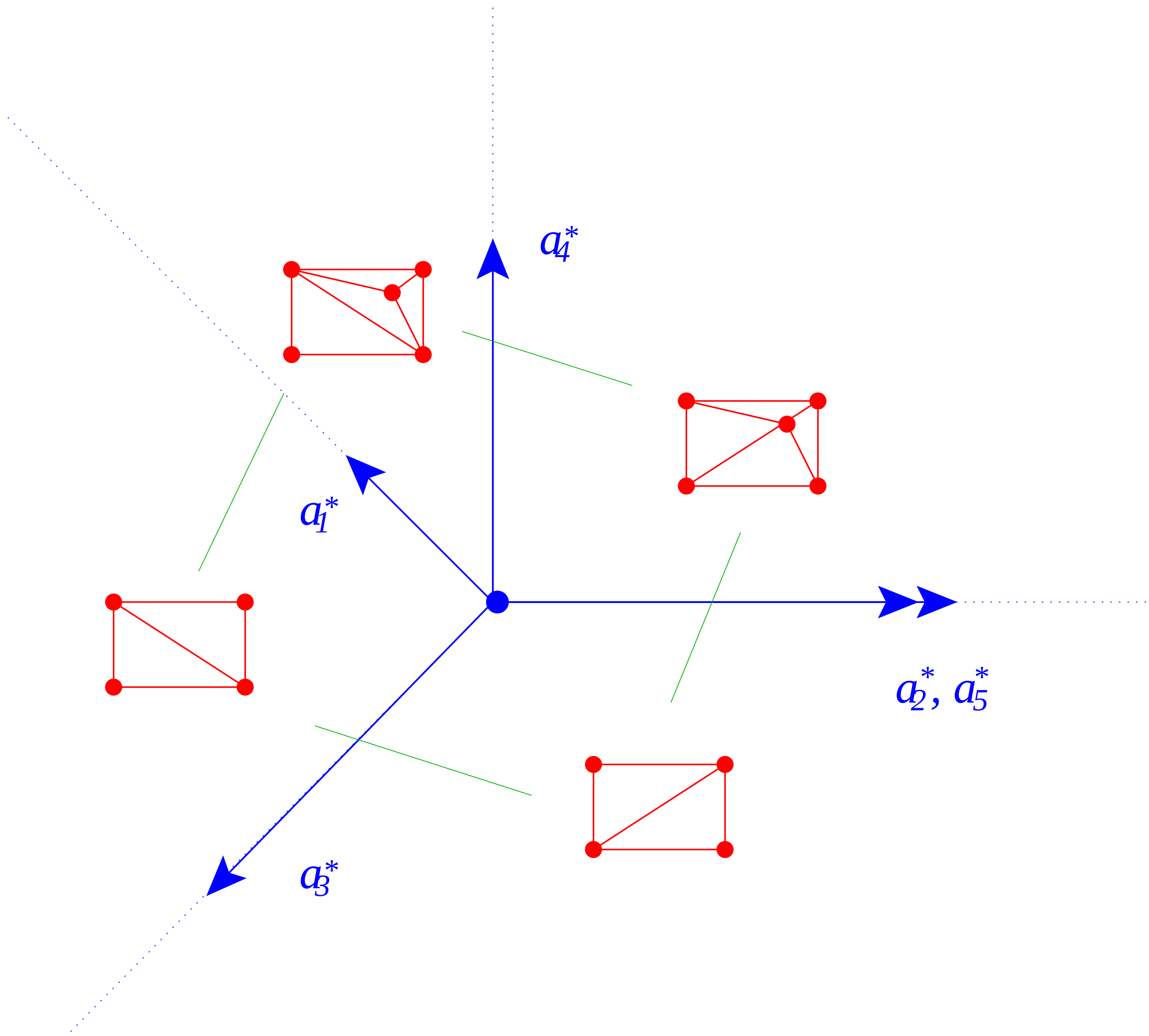
Consequently, we have

$$\begin{array}{ccccc} \mathcal{F}(\mathcal{A}) & = & RowSpace(A) & \times & \mathcal{F}'(\mathcal{A}) \\ \cap & & & & \cap \\ \mathbb{R}^n & = & RowSpace(A) & \times & ColSpace(G) \\ & & \cong \mathbb{R}^d & & \cong \mathbb{R}^{n-d} \end{array}$$



THEOREM (Billera, Filliman, Sturmfels 1990)

The fan $\mathcal{F}'(\mathcal{A})$ in the column space of A^* is the common refinement of all simplicial cones spanned by linearly independent subsets of $\mathcal{A}^*$.

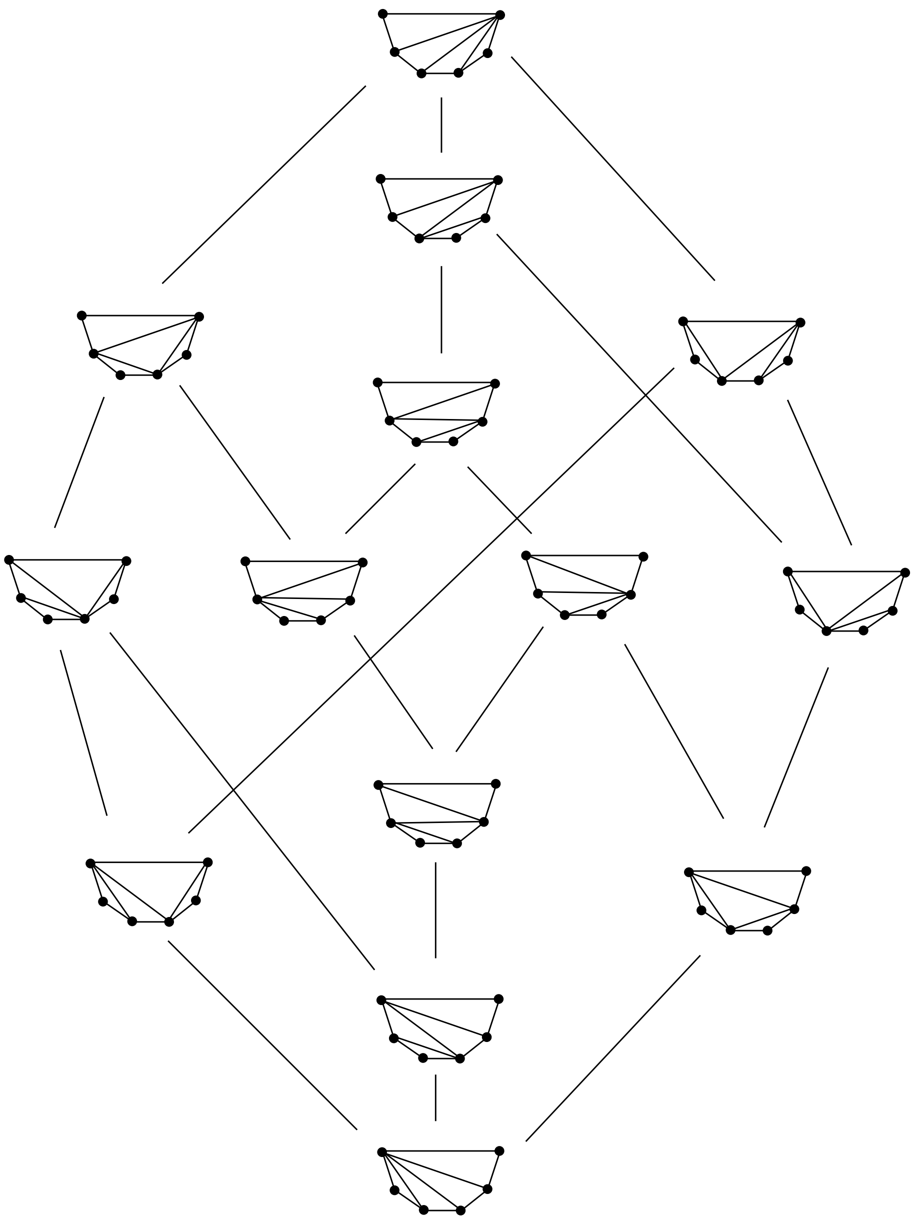


THEOREM (Gelfand, Kapranov, Zelevinsky 1990)

The fan $\mathcal{F}'(\mathcal{A})$ is actually the normal fan of an n-d-dimensional convex polytope, called the secondary polytope.

Hence the triangulations of $\mathcal{A}$ and the bistellar operations connecting them form the vertices and edges of the secondary polytope.

EXAMPLE: The associahedron
(J. Stasheff 1962, M. Haiman, C. Lee 1985):
$\mathcal{A}$ is the vertex set of a convex m-gon
($m = 6$ shown below).



Digression:
The Gale transform is closely related to

oriented matroid/ linear programming duality.

There is an oriented matroid represented by the affine point configuration $\mathcal{A}$, and $\mathcal{A}^*$ represents the dual oriented matroid.

One way to express this:

circuits in $\mathcal{A}$
(=sign patterns of coefficients
in minimal affine dependencies)

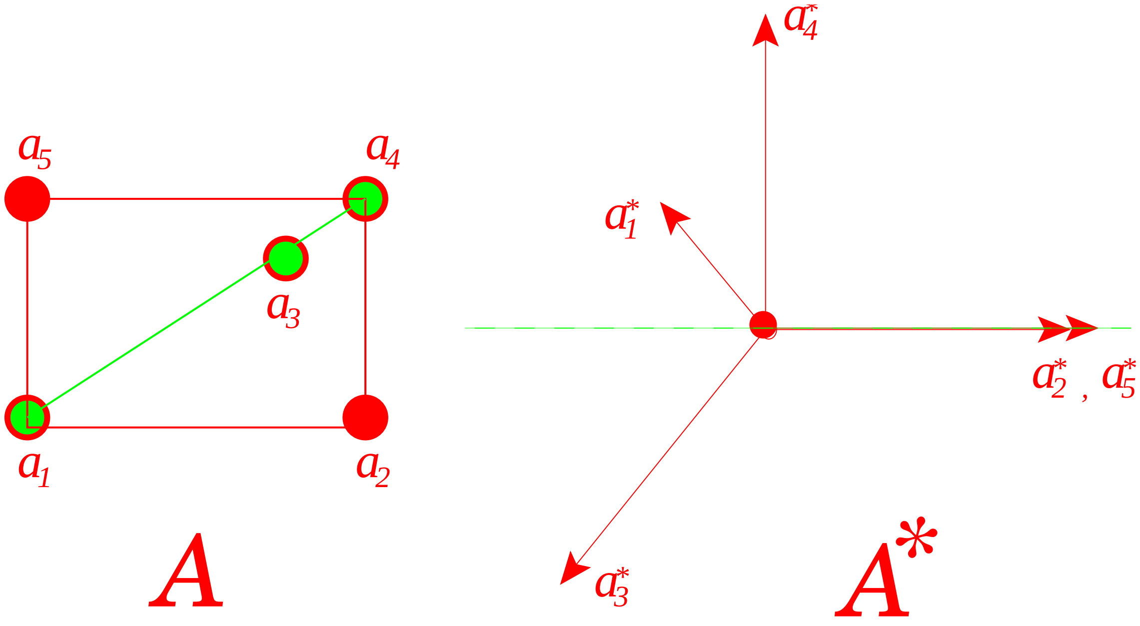
$$=$$

cocircuits in $\mathcal{A}^*$
(=sign patterns of values of linear functionals
vanishing on "almost all" vectors)

For example,

$$\begin{matrix} 1 & 2 & 3 & 4 & 5 \\ + & 0 & - & + & 0 \end{matrix}$$

is a circuit of $\mathcal{A}$ and a cocircuit of $\mathcal{A}^*$, as shown:

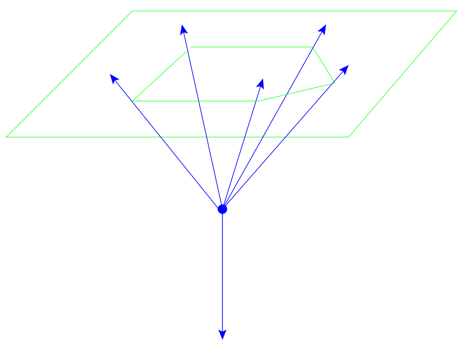


Some terminology:

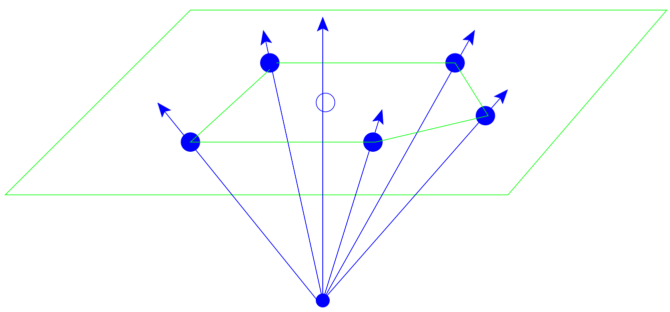
Gale transform (hard to visualize)

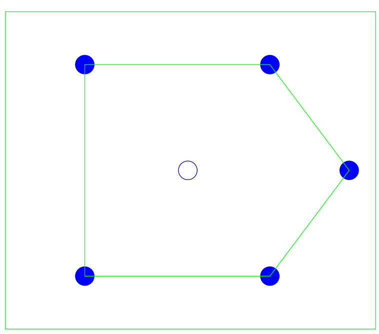
$$A^* = \begin{bmatrix} 2 & 1 & -1 & -1 & 1 & 0 \\ 0 & 1 & 1 & -1 & -1 & 0 \\ 1 & 1 & 1 & 1 & 1 & -1 \end{bmatrix}$$

Gale diagram (OK for $n - d \leq 2$)



affine Gale diagram (better for $n - d \geq 3$)





Other uses of Gale diagrams:

- "Visualizing", manipulating, and classifying polytopes with few vertices, that is, polytopes with n-d small (Gale 1956).

- Encoding matroid pathologies within polytopes, e.g.

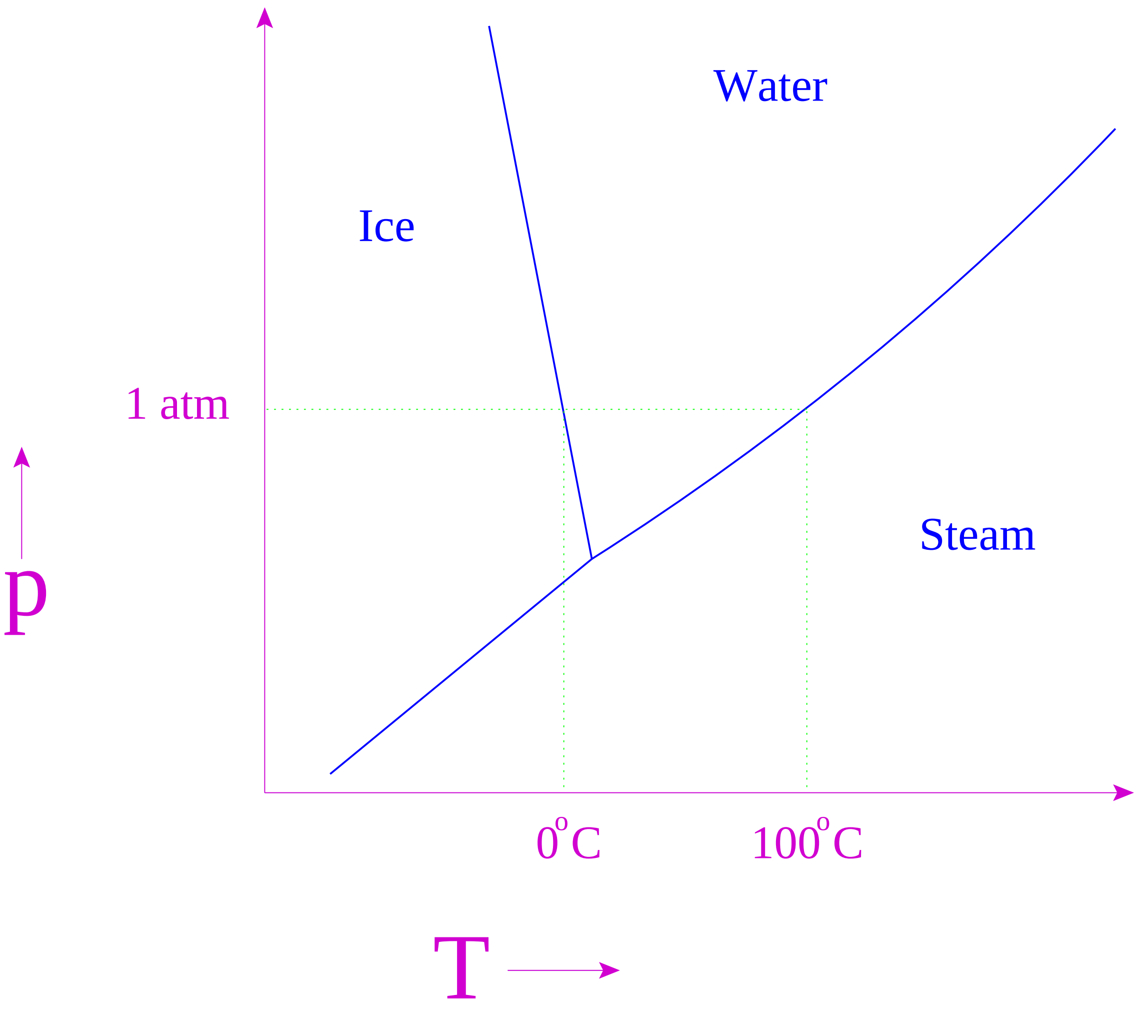
  - ▷ construction of non-rational polytopes (Perles 1967),

  - ▷ the Lawrence construction (Lawrence 1980?)

II. Geology

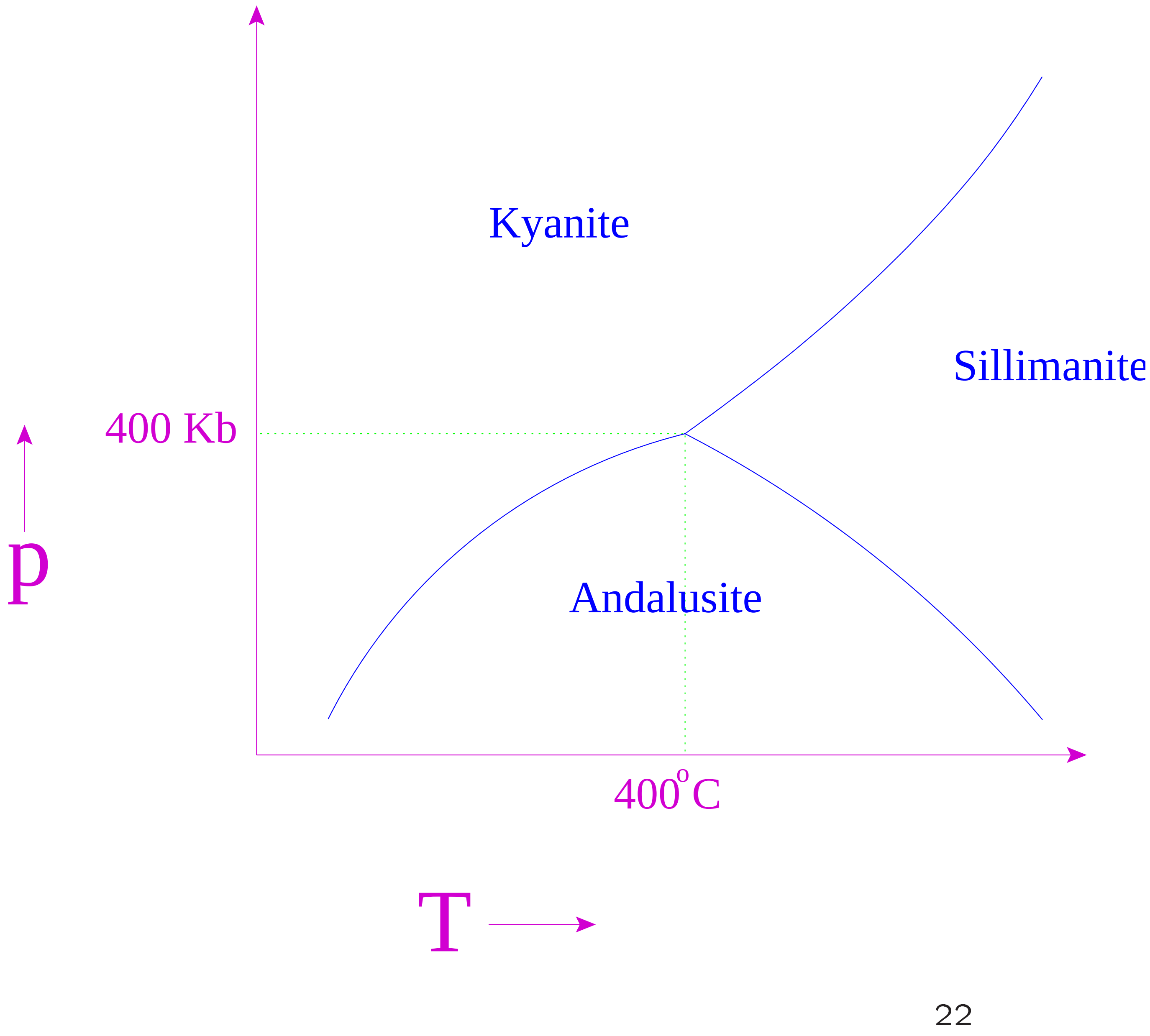
A familiar temperature-pressure (p, T) phase-diagram, involving the three phases of

$$H_2O$$



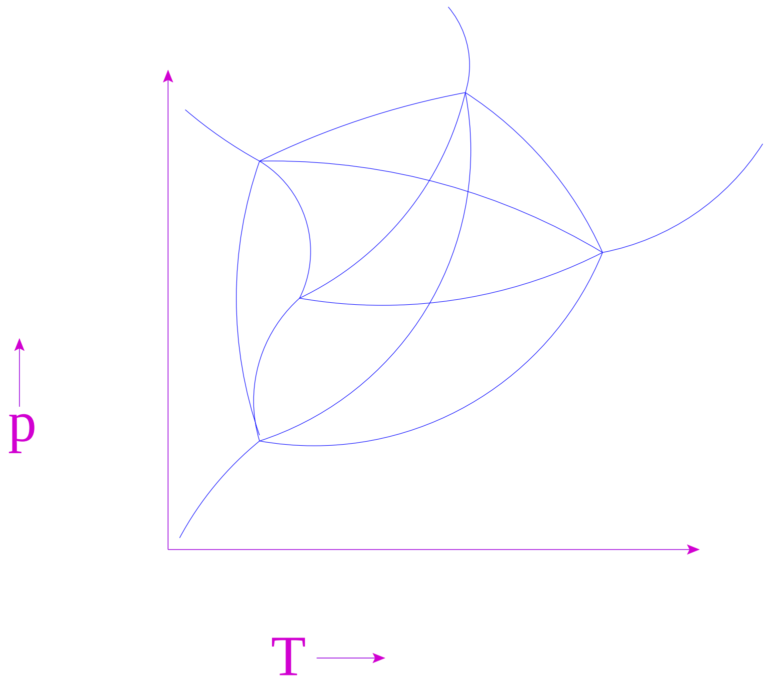
A more useful phase diagram for geologists, involving the three phases of Aluminum silicate

$$Al_2SiO_5$$



They get much complicated, particularly if the phases have more than one chemical formula, so reactions are possible.

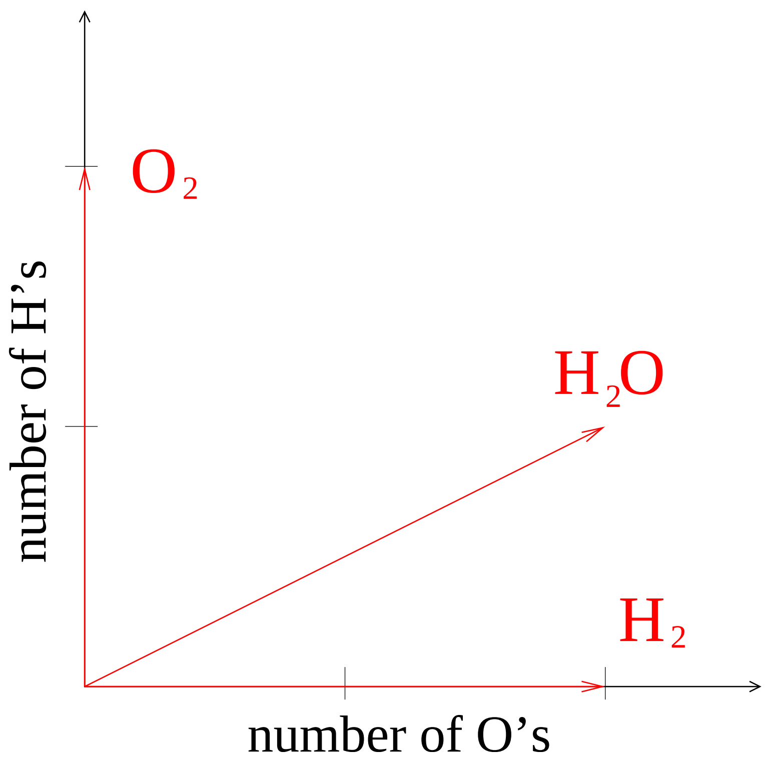
GOAL: Predict the possible combinatorics/topology of the phase diagram.



How to predict? If one plots chemical formulae of phases as vectors in chemcial composition space,

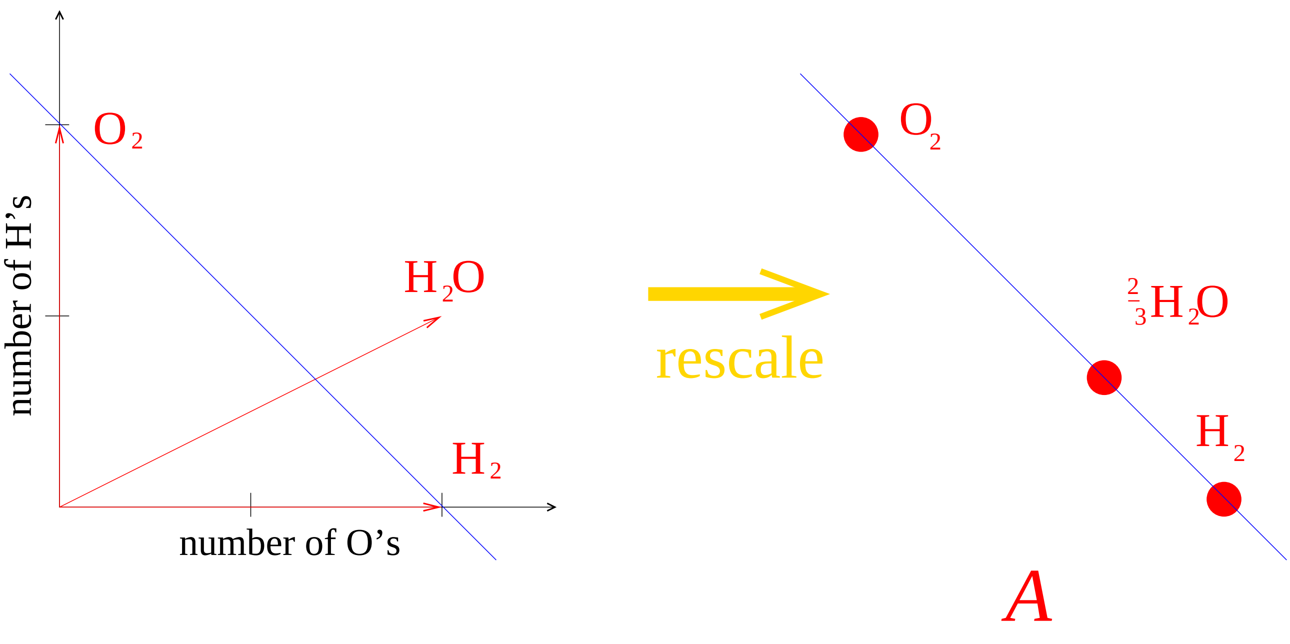
reactions = linear dependencies

$$2\,H_2 + 1\,O_2 \leftrightarrow 2\,H_2O$$



Rescale to get an affine point configuration $\mathcal{A}$,
and reactions become affine dependencies.

$$\frac{2}{3}H_2 + \frac{1}{3}O_2 \leftrightarrow 1\,\frac{2}{3}H_2O$$



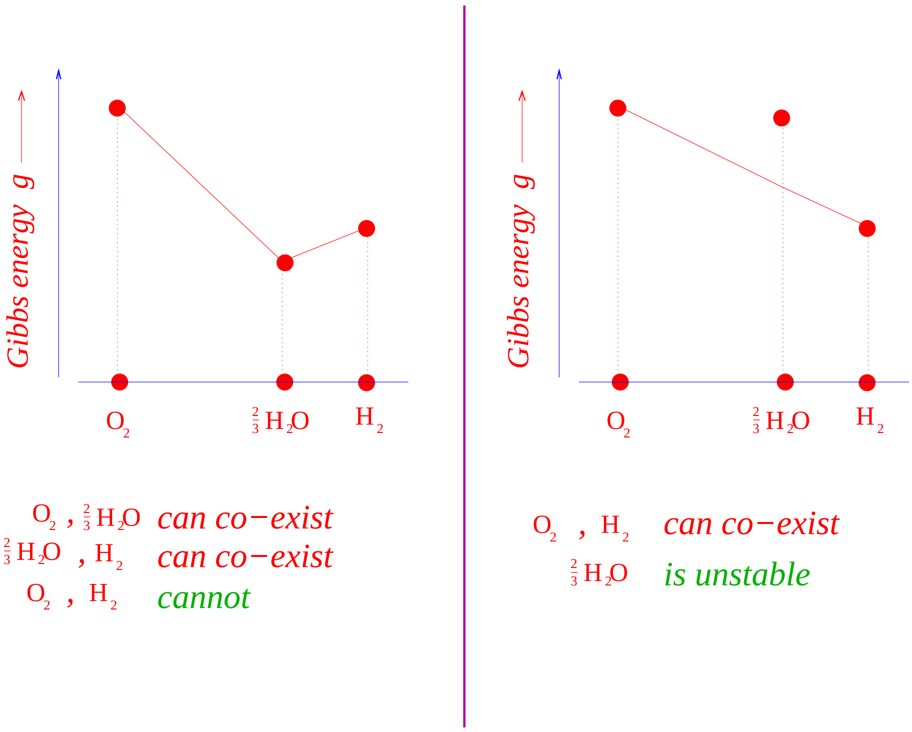
At a particular (p, T), which phases might I expect to find *stably* co-existing?

Each phase O_2, H_2, $\frac{2}{3}H_2O$ has its own Gibbs free energy

$$g_{O_2}(p,T),\ g_{H_2}(p,T),\ g_{\frac{2}{3}H_2O}(p,T)$$

and nature wants to minimize the *total* free energy.

Two possibilities:



From now on, assume we have

- n phases $\{a_1, \ldots, a_n\}$, and
- their chemical formulae span a d-dimensional space.

Let $\mathcal{A}$ be the associated point configuration in $\mathbb{R}^{d-1}$.

CONCLUSION 1

At a particular (p, T), Nature computes the coherent triangulation $\Delta(g)$ of $\mathcal{A}$ which is induced by the lifting vector

$$g = (g_{a_1}(p, T), \ldots, g_{a_n}(p, T)) \in \mathbb{R}^n,$$

in the following sense: the possible stably coexisting assemblages of phases are the simplices in $\Delta(g)$.

The combinatorics/topology of the (p, T) phase diagram?

Consider the map

$$\begin{array}{ccc} \mathbb{R}^2 & \xrightarrow{\gamma} & \mathbb{R}^n \\ (p, T) & \longmapsto & g = (g_{a_i}(p, T))_{i=1}^n \end{array}$$

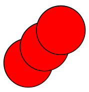
and its image $\mathrm{im}(\gamma)$ as a *parametrized surface* in $\mathbb{R}^n$.

Recall that $\mathbb{R}^n$ is decomposed into polyhedral cones by the secondary fan. This decomposition will then decompose the surface $\mathrm{im}(\gamma)$ in $\mathbb{R}^n$ into various regions.

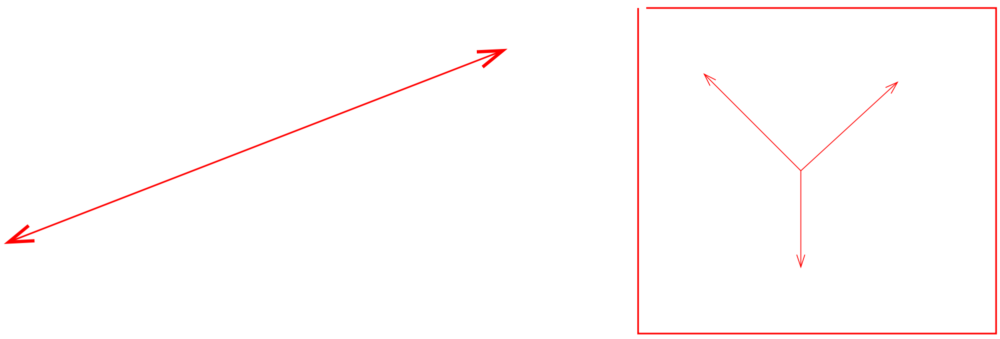
CONCLUSION 2

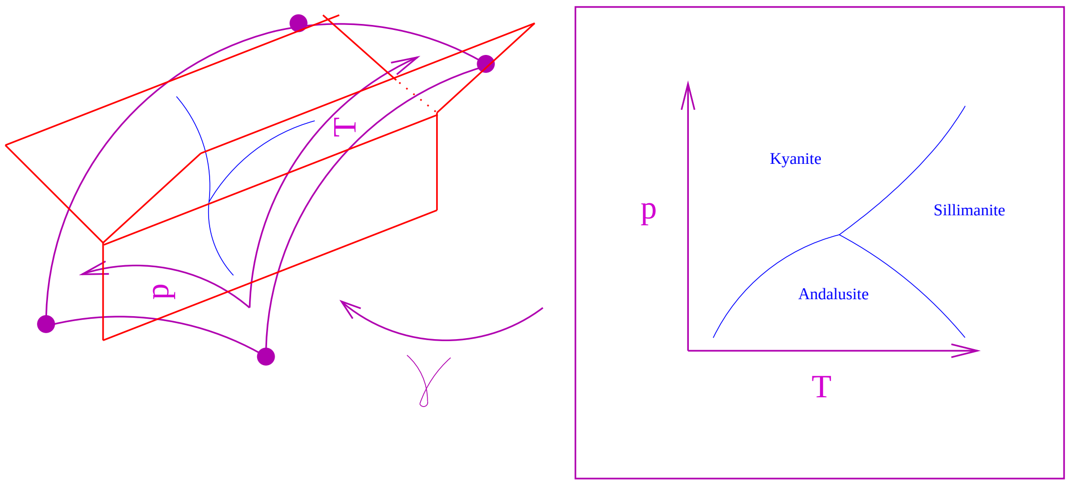
The (p, T) phase diagram is the pullback of this decomposition from the surface $\mathrm{im}(\gamma)$ to $\mathbb{R}^2$.

EXAMPLE: Kyanite (Al_2SiO_5), Sillimanite (Al_2SiO
Andalusite (Al_2SiO_5) has n $=$ 3 and d $=$ 1.

$A =$ 

$F(A) = Row(A) \oplus F'(A)$



$=$ 

GEOLOGISTS' IMPLICIT ASSUMPTION:

The map

$$\begin{array}{ccc} \mathbb{R}^2 & \xrightarrow{\gamma} & \mathbb{R}^n \\ (p,T) & \longmapsto & g = (g_{a_i}(p,T))_{i=1}^n \end{array}$$

- has nice monotonicity properties (e.g. it is in particular, one-to-one)

- is close to linear, so the surface im(γ) looks roughly like an affine 2-dimensional plane in $\mathbb{R}^n$.

- this 2-dimensional plane is transverse to Row(A).

CONCLUSION 3

When n-d = 2, we have roughly that

$$(p, T) \text{ phase diagram} = \text{Gale diagram } \mathcal{A}^* \ .$$

Schreinemakers rules 1911:

Gives rules for sketching the (p, T) phase diagram (= $\mathcal{A}^*$) when n-d = 2, given the reactions possible (=circuits) in $\mathcal{A}$.

His rules basically say

$$\text{circuits in } \mathcal{A} = \text{cocircuits in } \mathcal{A}^*$$

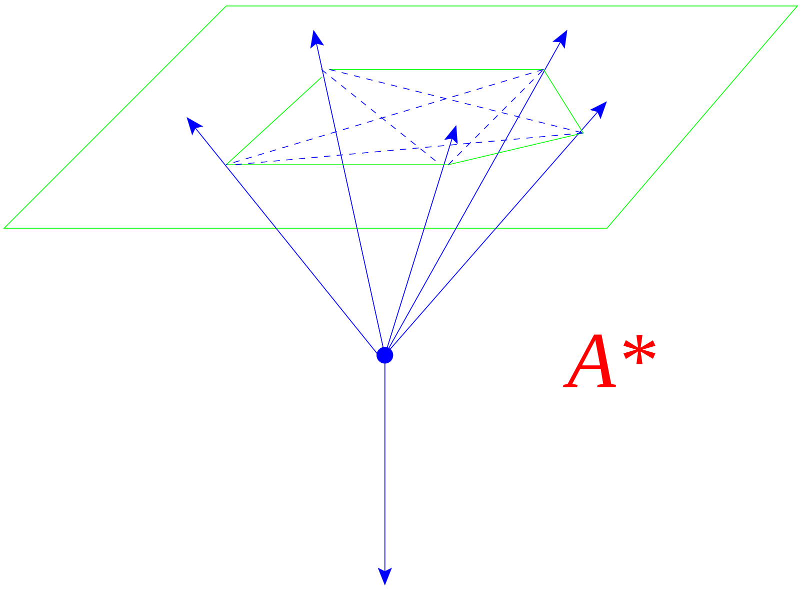
CONCLUSION 4

When n-d $= 3$, we have roughly that

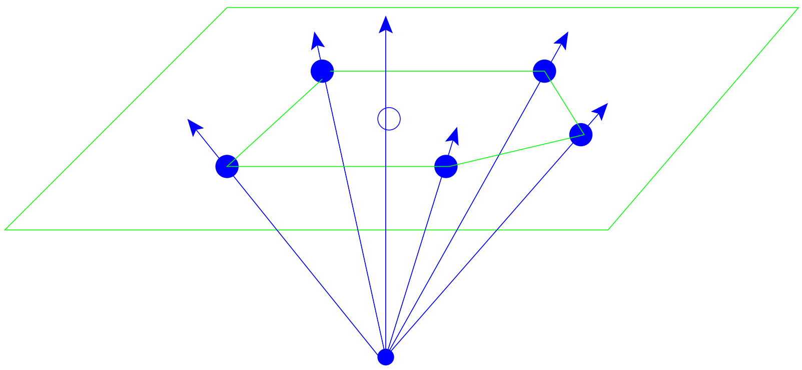
(p, T) phase diagram $=$
an affine Gale diagram for $\mathcal{A}^*$.

The choice of *which* Gale diagram is determined by where the affine 2-dimensional plane im(γ) lands in the pointed secondary fan $\mathcal{F}'(\mathcal{A})$.

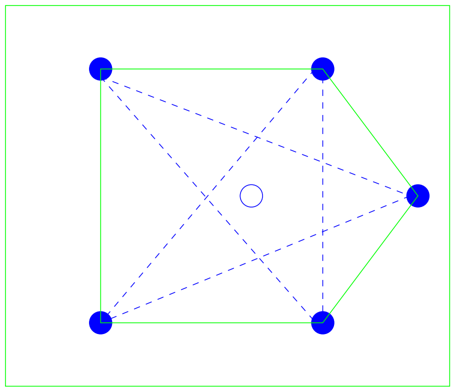
The different possible choices are parametrized by the vertices of a zonotope or the regions of a hyperplane arrangement.

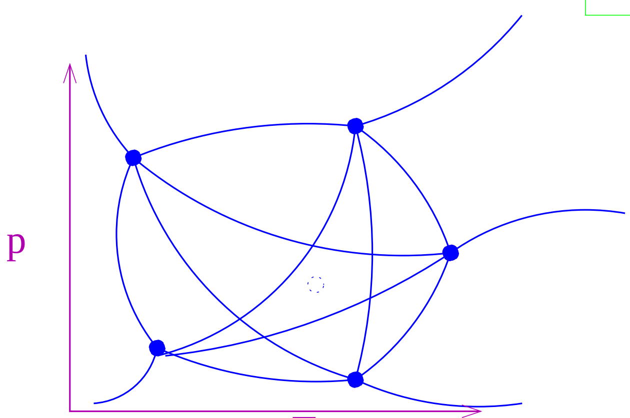


*A**



an affine Gale diagram





Where can math help?

- Automate the process of enumerating triangulations of $\mathcal{A}$, pointing out the incoherent ones, utilizing code by J. DeLoera, J. Rambau, connectivity results by C.L. Lawson 1977 ($d = 2$), Azaola and Santos 2000 ($n\text{-}d \leq 3$).

- Automate the possible choices of affine Gale diagram when $n\text{-}d = 3$, via theory of hyperplane arrangements.

The previous two goals were implemented in S. Peterson's Masters Thesis. See-
www.math.umn.edu/~reiner/CHEMOGALE.html.

Further help from math?

- Prove more connectivity results.

- Understand better how to parametrize choices of an affine 2-dimensional plane inside $\mathcal{F}'(\mathcal{A})$ for n-d > 3.

  In other words, how does $\mathcal{F}'(\mathcal{A})$ stratify the affine Grassmannian $\mathbf{G}r_{affine}(2, \mathbb{R}^{n-d})$?