

# Polyhedral geometry and algebra

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CTMS Retreat  
23 October 2009

## What kind of research do I do?

“Combinatorial aspects of geometry and algebra”

- algebra and combinatorics of polynomial systems
- topology and geometry of algebraic varieties (solution sets)
- continuous symmetry: Lie groups and representations
- symbolic computation with polynomials
- combinatorial games
- polyhedral metric spaces (combinatorics, computation, complexity)
  - unfolding (existence and algorithms)
  - discrete geodesic problems
  - flows and optimization
- connections with
  - physics: string theory [with Aspinwall, Plesser, Mapes]
  - biology: phylogenetics, evolution, imaging
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# Averaging phylogenetic trees

**Observation.** Gene histories do not agree with species histories

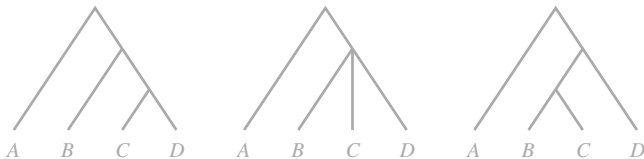
**Conclusion.** Gene trees are distributed randomly around species trees

**Current methods.** Details of evolutionary processes  
     $\rightsquigarrow$  heuristics for constructing phylogenies

**Hypothesis.** Law of large numbers  $\Rightarrow$  phylogeny = “average gene tree”

**Method.** Metric trees with  $n$  leaves is a “CAT(0)” polyhedral space

- e.g., fixed tree topology  $\Rightarrow$  orthant = {lists of edge lengths}



- not a manifold, but “negatively curved” nonetheless
- means of probability distributions make sense [Sturm 2003]

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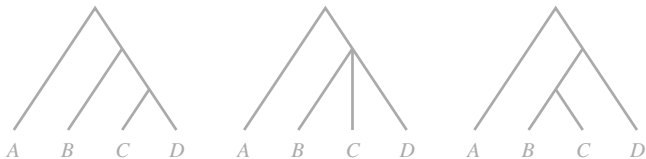
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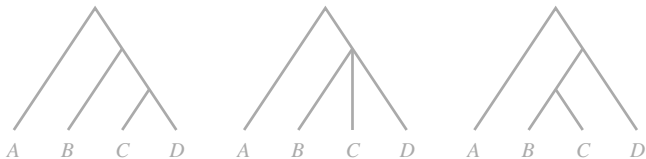
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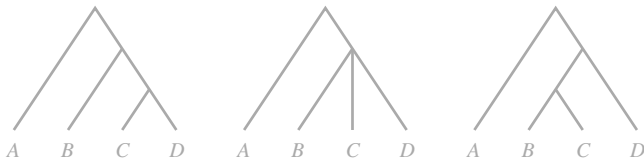
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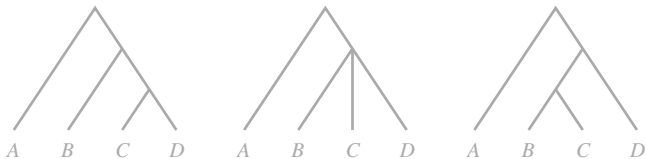
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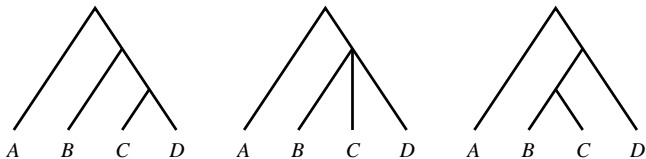
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- polyhedral subdivision according to combinatorial type of path
- convex optimization on an appropriate cell

**Biology.** Need data sets from multiple species with

- known phylogenies
- sufficiently large numbers of known gene trees

**Brain imaging.** Tree  $\leftrightarrow$  arterial structure

- detect clustering
- calculate best fits (best fit point = centroid; best fit line = ?)
- general: statistics on polyhedral spaces? (not topological manifolds!)

**Further math.**

- optimization on general (non-manifold) polyhedral spaces
- gradient vector fields for splines

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# Mass-action kinetics

[Guldberg and Waage, 1864]

- chemical species  $s_1, \dots, s_n$  with concentrations  $[s_i] = x_i = x_i(t)$
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$$\dot{x}_i = (b_i - a_i)(\lambda \mathbf{x}^{\mathbf{a}} - \mu \mathbf{x}^{\mathbf{b}}) \quad \text{for some rate constants } \lambda, \mu > 0.$$

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**Definition.** The system is **detailed balanced** if the binomials in (\*) simultaneously vanish at a point in  $\mathbb{R}^n$  with strictly positive entries.

**Conjecture (Global Attractor Conjecture [Horn-Jackson 1972])**

*If the differential system (\*) has a detailed balanced equilibrium, then all trajectories with positive initial conditions reach it in the limit.*

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$$\dot{\mathbf{x}} = \sum_{\mathbf{a} \rightleftharpoons \mathbf{b}} (\mathbf{b} - \mathbf{a})(\lambda_{\mathbf{ab}} \mathbf{x}^{\mathbf{a}} - \lambda_{\mathbf{ba}} \mathbf{x}^{\mathbf{b}}). \quad (*)$$

**Definition.** The system is **detailed balanced** if the binomials in (\*) simultaneously vanish at a point in  $\mathbb{R}^n$  with strictly positive entries.

**Conjecture (Global Attractor Conjecture [Horn-Jackson 1972])**

*If the differential system (\*) has a detailed balanced equilibrium, then all trajectories with positive initial conditions reach it in the limit.*

**Mathematics.** Commutative algebra of binomials controls dynamics  
[with Manoj Gopalkrishnan (Tata, Mumbai) and Anne Shiu (UC Berkeley)]

# Mass-action kinetics

[Guldberg and Waage, 1864]

- chemical species  $s_1, \dots, s_n$  with concentrations  $[s_i] = x_i = x_i(t)$
- chemical complexes  $A = a_1 s_1 + \dots + a_n s_n$  and  $B = b_1 s_1 + \dots + b_n s_n$
- concentrations  $[A] = \mathbf{x}^{\mathbf{a}} = x_1^{a_1} \dots x_n^{a_n}$  and  $[B] = \mathbf{x}^{\mathbf{b}} = x_1^{b_1} \dots x_n^{b_n}$
- reversible reaction  $A \rightleftharpoons B$  evolves under **mass action kinetics** if

$$\dot{x}_i = (b_i - a_i)(\lambda \mathbf{x}^{\mathbf{a}} - \mu \mathbf{x}^{\mathbf{b}}) \quad \text{for some rate constants } \lambda, \mu > 0.$$

- For multiple reactions, sum:

$$\dot{\mathbf{x}} = \sum_{\mathbf{a} \rightleftharpoons \mathbf{b}} (\mathbf{b} - \mathbf{a})(\lambda_{\mathbf{ab}} \mathbf{x}^{\mathbf{a}} - \lambda_{\mathbf{ba}} \mathbf{x}^{\mathbf{b}}). \quad (*)$$

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