Phylogenetic invariants and tensors of border rank 4 at most in $\mathbb{C}^{4 \times 4 \times 4}$

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ILAS meeting in Pisa, 22 June, 2010
Summary

1. Phylogenetic trees and their invariants
2. Statement of the problem
3. Border rank
4. Known results
5. New conditions
6. Outline of the complete solution
Phylogenetic Tree of Life

Bacteria
- Spirochetes
- Proteobacteria
- Cyanobacteria
- Planctomyces
- Bacteroides
- Cytophaga
- Thermotoga
- Aquifex

Archaea
- Green filamentous bacteria
- Gram positives
- Methanococci
- Methanosarcina
- Thermoproetus
- Pyrodictium

Eucaryota
- Entamoebae
- Slime molds
- Animals
- Fungi
- Plants
- Ciliates
- Flagellates
- Trichomonads
- Microsporidia
- Diplomonads
Reconstruction of the Phylogenetic tree with $n$ taxa

Given $n$ leaves of a tree, taxa

Find a best tree with internal vertices of degree 3 with given taxa

Branching pattern of the tree is called the topology

The evolution of the tree is modeled by Markov chain

Evolution: random substitution of one nucleotide of DNA $A$, $G$, $C$, $T$ at individual sites

The topology of the tree gives rise to the joint distribution of the taxa $X = (X_1, \ldots, X_n)$, $X_i \in \{A, G, C, T\} = \{1, 2, 3, 4\}$, $i = 1, \ldots, n$

Joint distribution of $X$ is tensor $T = \left[ t_{i_1 \ldots i_n} \right] \in \otimes_n [0, 1]$

Basic problem of algebraic statistics:

Characterize the variety which is a closure of all $T$ corresponding to a given tree

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One parent, (the root) 3 descendants, (taxa): $x, y, z$
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$$\mathcal{T} = \pi_A x_A \otimes y_A \otimes z_A + \pi_C x_C \otimes y_C \otimes z_C + \pi_G x_G \otimes y_G \otimes z_G + \pi_T x_T \otimes y_T \otimes z_T$$

$x_A, \ldots, z_T, \pi = (\pi_A, \pi_C, \pi_G, \pi_T)^\top$ probability vectors in $\mathbb{R}^4$
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$T \in \mathbb{C}^{4 \times 4 \times 4}$ has a border at most $k$
if it is a limit of tensors of rank $k$ at most
Ranks of tensor 1

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\( \text{grank}(m, n, l) = l \text{ for } l \in [(m - 1)(n - 1) + 1, l] \)

Reason: A generic space \( \mathbf{W} \subset \mathbb{C}^{m \times n}, \dim \mathbf{W} = (m - 1)(n - 1) + 1 \) intersects the variety of all matrices of rank 1: \( \mathbb{C}^{m \times n} \subset \mathbb{C}^{m \times n} \) at least \([(m - 1)(n - 1) + 1, l]\).
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Generic subspace $W \subset S(m, \mathbb{C})$, $\dim W = \frac{m(m-1)}{2} + 1$ intersects variety of symmetric matrices of rank 1 at least at $\frac{m(m-1)}{2} + 1$ lin. ind. mat.

Cor.: generic $\mathcal{T} \in \mathbb{C}^{3 \times 3 \times 4}$ symmetric in the first two indices has rank 4
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Strassen 1983: a. $\text{grank}(3, 3, 3) = 5$
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b. variety of all tensors in $\mathbb{C}^{3 \times 3 \times 3}$ of at most rank 4 is a hypersurface of degree 9

$$\frac{1}{\det Z} \det \left( X(adj Z) Y - Y(adj Z) X \right) = 0$$

$X, Y, Z$ are three sections of $\mathcal{T}$
Tensors of rank $m$ in $\mathbb{C}^{m \times m \times l}$
Tensors of rank \( m \) in \( \mathbb{C}^{m \times m \times l} \)

\( \mathcal{T} \in \mathbb{C}^{m \times m \times l} \), \( \text{rank } \mathcal{T} = m \), \( \mathbf{W} = \text{span}(T_{1,3}, \ldots, T_{l,3}) \in \mathbb{C}^{m \times m} \)

spanned by \( \mathbf{u}_1 \mathbf{v}_1^\top, \ldots, \mathbf{u}_m \mathbf{v}_m^\top \).
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Generic case: $\exists P, Q \in \text{GL}(m, \mathbb{C})$ $P W Q$ subspace of commuting diagonal matrices $\iff Z^{-1} W$ a subspace of commuting matrices.
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If $W$ contains an invertible matrix $Z$ then any other $X, Y \in W$ satisfy $X(\text{adj}Z)Y = Y(\text{adj}Z)X$ - equations of degree 5 for $m = 4$
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Strassen’s condition hold for any $3 \times 3 \times 3$ subtensor of $\mathcal{T} \in \mathbb{C}^{4 \times 4 \times 4}$: equations of degree 9
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equations of degree 9

[3] one needs equations of degree 16
Manivel-Landsberg to determine completely the variety of tensors of border rank at most 4 in $\mathbb{C}^4 \times \mathbb{C}^4 \times \mathbb{C}^4$ one needs in addition to above conditions to determine the the variety of tensors of border rank at most 4 in $\mathbb{C}^3 \times \mathbb{C}^3 \times \mathbb{C}^4$:

$$\text{span}(u_1v_1^\top, \ldots, u_4v_4^\top)$$

where any three vectors out of $u_1, \ldots, u_4$ and $v_1, \ldots, v_4$ linearly independent.

$\exists P, Q \in \text{GL}(3, \mathbb{C})$:

$$Pu_i = Qv_i = (\delta_{i1}, \delta_{i2}, \delta_{i3})^\top, \quad i = 1, 2, 3,$$

$$Pu_4 = Qv_4.$$

$\iff P W Q \subset S(3, \mathbb{C}) \iff \exists 0 \neq S, T \in \mathbb{C}^{3 \times 3}$ s.t.

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generic subspace spanned by four rank one matrices in $C^{4 \times 4}$: 
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$\iff PWQ \subset S(3, \mathbb{C})$  
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$SW_i - W_i^T S^T = 0, \ i = 1, \ldots, 4, \quad W_i T - T^T W_i^T = 0, \ i = 1, \ldots, 4$

existence of nontrivial solutions $S, T$, each system in 9 variables, (entries of) $S, T$ implies that any $9 \times 9$ minor of the coefficient matrix of two systems vanishes
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expressing all possible solutions $S, T$ in terms of $8 \times 8$ minors of coefficient matrices, the conditions $ST = TS = \lambda I$ are given by vanishing of the corresponding $16$–$th$ degree polynomials
Sufficiency of all conditions

If $W \subset \mathbb{C}^{4 \times 4}$, $\dim W = 4$ contains an invertible matrix then commutativity conditions $X(adj Z)Y - Y adj(Z)X = 0$ imply that border rank of $T \in \mathbb{C}^{4 \times 4 \times 4}$ at most 4.

need to use fact: variety of commuting matrices $(A_1, A_2, A_3) \subset (\mathbb{C}^{3 \times 3})^3$ is irreducible [4]
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If subspace spanned by each $p = 1, 2, 3$ sections of $T$ does not contain an invertible matrix then by change of basis in each factor and possibly permute the factors $T \in \mathbb{C}^{3 \times 3 \times 4}$. 
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$W = \text{span}(T_{1,3}, \ldots, T_{4,3}) \subset \mathbb{C}^{3 \times 3}$. If $\dim W \leq 3$ use Strassen’s condition $\dim W = 4$ use symmetrization condition. If $S$ or $T$ invertible $\text{brank} T \leq 4$.

If $S$, $T$ singular, analyze different cases to show that $\text{brank} T \leq 4$.

Some of them use the 16 degree condition


S. Friedland, On tensors of border rank $l$ in $\mathbb{C}^{m \times n \times l}$, arXiv:1003.1968v1.

