Toric Ideals of Phylogenetic Invariants for the General Group-based Model

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Outline

- Motivation:

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  Statistical models of evolution

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- Main Theorem and consequences

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- Ideals of phylogenetic invariants

- Main Theorem and consequences

- What next...

Motivation

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Figure: Pictures by Marta Casanellas

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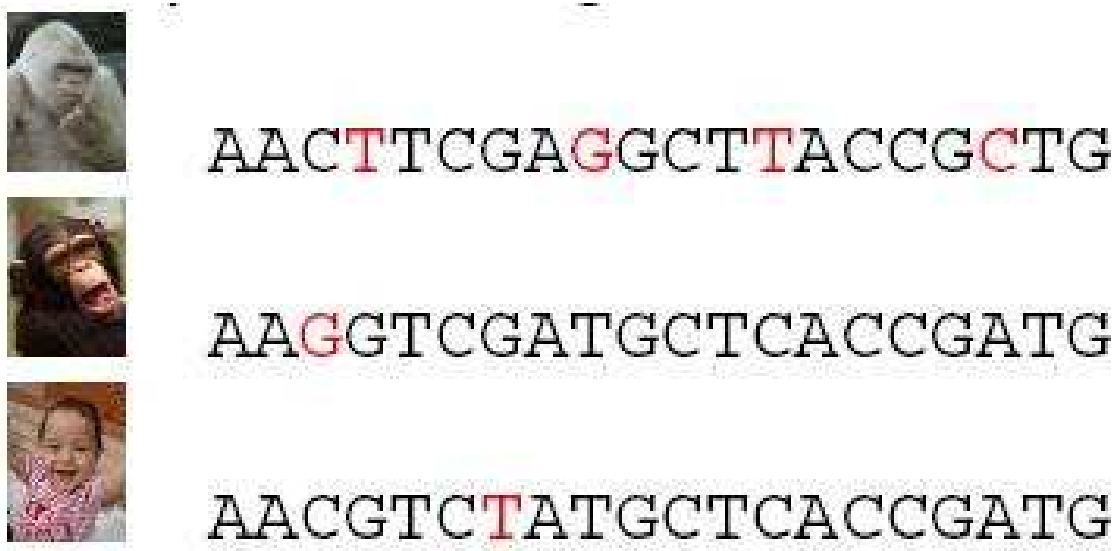

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- Phylogenetic algebraic geometry picture:
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- Application
  Use phylogenetic ideals to determine genetic relationship between species based on their DNA sequences.

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construct the phylogenetic tree corresponding to the given species.

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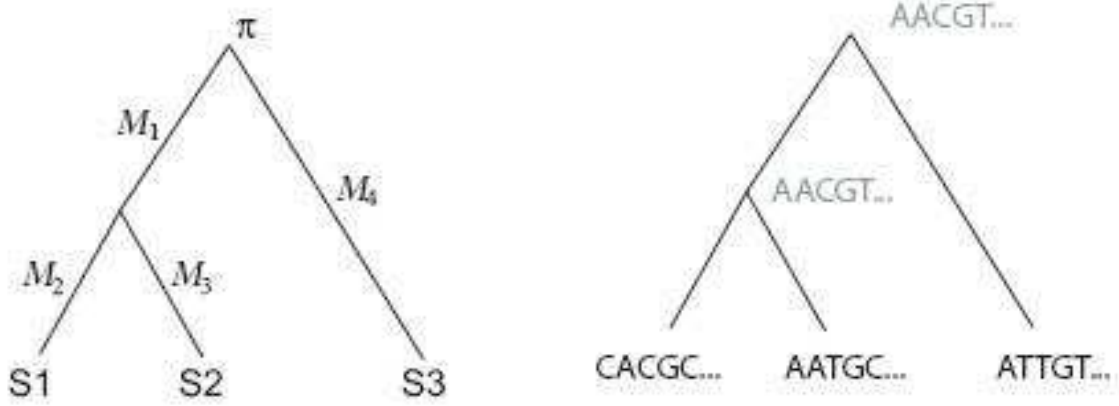

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- A possible alignment is:
  seq1 : A C – G – T A – G C T A A G T T A
  seq2 : A C C G A G A C – C C A – G T – A
  seq3 : A C C A A G A C A – C A – G T – A...

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$$\hat{p}_{GGA} = \frac{\text{number of observations of GGA}}{\text{sequence length}}$$

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- Know the true p for a model and a tree $\Longrightarrow$ plug in data to check if model/tree correct!

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- p_σ is a polynomial in the model parameters.

Example: find true probabilities for a given tree

T = tree on 2 leaves.

Suppose root has uniform distribution: $p_{rA} = p_{rG} = p_{rC} = p_{rT} = 1/4$.

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- Edge transition matrix $M_e = \begin{bmatrix} p_{A|A} & p_{A|G} & p_{A|C} & p_{A|T} \\ p_{G|A} & p_{G|G} & p_{G|C} & p_{G|T} \\ p_{C|A} & p_{C|G} & p_{C|C} & p_{C|T} \\ p_{T|A} & p_{T|G} & p_{T|C} & p_{T|T} \end{bmatrix}$

- $p_{AG} = 1/4 p_{rA} p_{A|A} p_{G|A} + 1/4 p_{rG} p_{A|G} p_{G|G} + 1/4 p_{rC} p_{A|C} p_{G|C} + 1/4 p_T p_{A|T} p_{G|T}$

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Goal

Understand all the polynomials p_σ for any tree on n leaves.

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Definition

Ideal of phylogenetic invariants = $\ker \phi$.

Computing this ideal is hard!

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- Examples: Jukes-Cantor, Kimura's one-parameter models used in computational biology.

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Fact

Every group-based model is a specialization of the general group-based model.

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the ideal of phylogenetic invariants for the tree T_n is the kernel of the following homomorphism between polynomial rings:

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$$q_{g_1,\ldots,g_n} \mapsto a_{g_1}^{(1)} a_{g_2}^{(2)} \ldots a_{g_n}^{(n)} a_{g_1+g_2+\cdots+g_n}^{(n+1)},$$

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The coordinate $q_{g_1,\ldots,g_n}$ corresponds to observing the element g_1 at the first leaf of T, g_2 at the second, ...

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- For the group $\mathbb{Z}_2$ on any claw tree, we:

  describe explicitly the lattice basis ideal

  and a quadratic Gröbner basis of the ideal of invariants (without using saturation).

Example: $n = 3$

$$\varphi : q_{000} \mapsto a_0^{(1)} a_0^{(2)} a_0^{(3)} a_{0+0+0}^{(4)} \qquad q_{100} \mapsto a_1^{(1)} a_0^{(2)} a_0^{(3)} a_{1+0+0}^{(4)}$$

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φ represented by

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 & 1 & 0 & 0 & 1 \end{bmatrix}$$

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$\dim \ker(\text{ matrix of } \varphi) = 3$.

The lattice basis is given by the rows of:

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Already saturated, thus equals ideal of invariants.
Let $q_{000} > q_{001} > q_{010} > q_{011} > q_{100} > q_{101} > q_{110} > q_{111}$.

Remark

The three generators of I_3 above are a lexicographic Gröbner basis for I_3 , since the initial terms, written with coefficient $+1$ in the above description, are relatively prime so all the S-pairs reduce to zero.

Example: $n = 4$

Ideal of invariants for the 4-leaf claw tree:

$$q_{0000}q_{0111} - q_{0100}q_{0011},\ q_{0001}q_{0110} - q_{0100}q_{0011},\ q_{0010}q_{0101} - q_{0100}q_{0011},$$
$$q_{0000}q_{1011} - q_{1000}q_{0011},\ q_{0001}q_{1010} - q_{1000}q_{0011},\ q_{0010}q_{1001} - q_{1000}q_{0011},$$
$$q_{0000}q_{1101} - q_{1000}q_{0101},\ q_{0001}q_{1100} - q_{1000}q_{0101},\ q_{0100}q_{1001} - q_{1000}q_{0101},$$
$$q_{0000}q_{1110} - q_{1000}q_{0110},\ q_{0010}q_{1100} - q_{1000}q_{0110},\ q_{0100}q_{1010} - q_{1000}q_{0110};$$
$$q_{1000}q_{1111} - q_{1100}q_{1011},\ q_{1001}q_{1110} - q_{1100}q_{1011},\ q_{1010}q_{1101} - q_{1100}q_{1011},$$
$$q_{0100}q_{1111} - q_{1100}q_{0111},\ q_{0101}q_{1110} - q_{1100}q_{0111},\ q_{0110}q_{1101} - q_{1100}q_{0111},$$
$$q_{0010}q_{1111} - q_{1010}q_{0111},\ q_{0011}q_{1110} - q_{1010}q_{0111},\ q_{0110}q_{1011} - q_{1010}q_{0111},$$
$$q_{0001}q_{1111} - q_{1001}q_{0111},\ q_{0011}q_{1101} - q_{1001}q_{0111},\ q_{0101}q_{1011} - q_{1001}q_{0111}.$$
$$q_{0000}q_{1111} - q_{1001}q_{0110},\ q_{0001}q_{1110} - q_{1000}q_{0111},\ q_{0011}q_{1100} - q_{1001}q_{0110},$$
$$q_{0010}q_{1101} - q_{1000}q_{0111},\ q_{0101}q_{1010} - q_{1001}q_{0110},\ q_{0100}q_{1011} - q_{1000}q_{0111}.$$

$2^4 = 16$ variables.
Ideal of invariants: 30 generators.
Lattice basis ideal: 10 generators.

Invariants for an arbitrary claw tree

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Theorem

For $n \geq 4$, $\quad I_n = (q : q^+ - q^- \in \mathcal{G}_n)$.
In addition, this set of generators can be obtained inductively by lifting the generators corresponding to the various phylogenetic ideals on $n-1$ *leaves.*

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Number of variables: 2^n. Number of ideal generators:
$\binom{2^n+1}{2} + \cdots + \binom{2^3+1}{2} - [3^n + \cdots + 3^3] - [\binom{2^{n-1}}{2} + \cdots + \binom{2^2}{2}]$.

Conclusion

- Combined with the main result of Sturmfels and Sullivant, this implies that the phylogenetic ideal of every tree for the group $\mathbb{Z}_2$ has a quadratic Gröbner basis.

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- Hence, the coordinate ring of the toric variety is a Koszul algebra.
- In addition, the ideals for every tree can be computed explicitly.
- We are working on extending these results to the group $\mathbb{Z}_2 \times \mathbb{Z}_2$.

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References: Nick Eriksson.

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References: Steve Feinberg; Yi Zhou.