Technische Universiteit
Eindhoven
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Bounded-rank tensors and group-based models

Jan Draisma
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27 September 2011

Tropical Geometry and
Computational Biology
Saarbrücken

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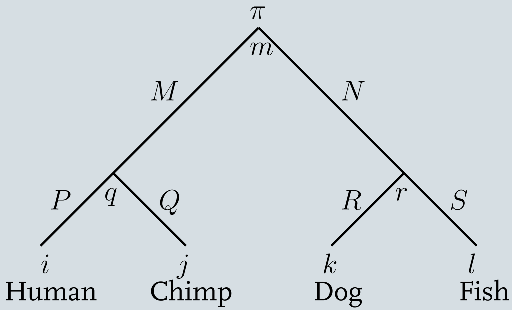
Tree models



$$\mathrm{Prob}(i,j,k,l) = \sum_{m,q,r} \pi_m M_{qm} P_{iq} Q_{jq} N_{rm} R_{kr} S_{lr}$$

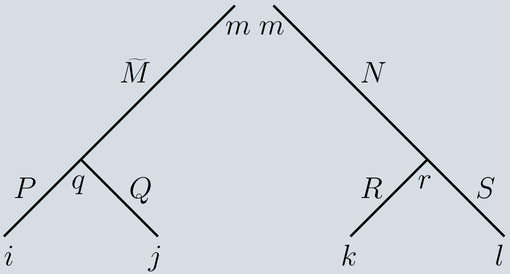
$$\mathrm{Prob} \in \mathbb{R}^{\{\mathrm{A,C,G,T}\}^p} = \mathbb{R}^{4\times\cdots\times 4}$$

p number of leaves

$$\mathrm{Model} = \{\mathrm{Prob} \mid \pi, M, \ldots, S\}$$

Products of star models

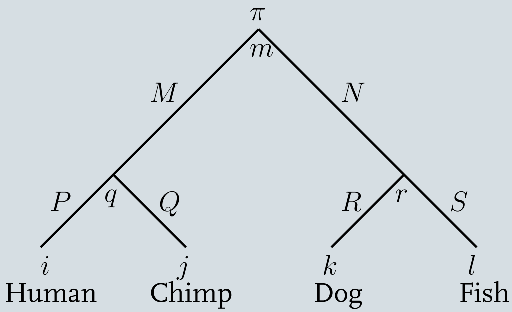
$$\mathrm{Prob}(\underbrace{i,j},k,l) = \sum_m (\sum_q \widetilde{M}_{qm} P_{iq} Q_{jq})(\sum_r N_{rm} R_{kr} S_{lr}) = \sum_m \mathrm{Prob}_1(i,j,m)\mathrm{Prob}_2(m,k,l)$$



$$\mathrm{Prob} = \mathrm{Prob}_1 \cdot \mathrm{Prob}_2$$
$$\mathrm{Model} = \mathrm{Model}_1 \cdot \mathrm{Model}_2$$

$$\mathrm{Model}_1, \mathrm{Model}_2 \subseteq \mathbb{R}^{\{\mathrm{A,C,G,T}\}^3}$$
$$\mathrm{Model} \subseteq \mathbb{R}^{\{A,C,G,T\}^p},\ p = 4$$

Tree models



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Products of star models

Prob$(i, j, k, l) = \sum_m$
$(\sum_q \widetilde{M}_{qm} P_{iq} Q_{jq})(\sum_r N_{rm} R_{kr} S_{lr}) =$
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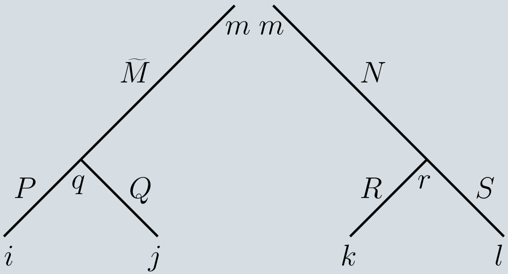


Prob $=$ Prob$_1 \cdot$ Prob$_2$
Model $=$ Model$_1 \cdot$ Model$_2$

Model$_1$, Model$_2 \subseteq \mathbb{R}^{\{\text{A,C,G,T}\}^3}$
Model $\subseteq \mathbb{R}^{\{A,C,G,T\}^p}$, $p = 4$

Phylogenetic invariants

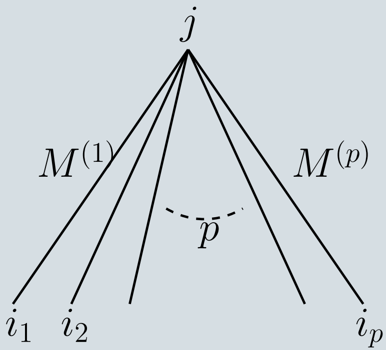
Does the tree fit the data?
1. ML-estimation
2. **equations** for Model
polynomial ideal in 4^p variables

Many contributors:
Allman, Casanellas, Pachter,
Rhodes, Sturmfels, Sullivant, ...

Allman-Rhodes, D-Kuttler:
Description of ideal I(Model)
from $I(\text{Model}_1)$, $I(\text{Model}_2)$.

Equations for stars?

Stars and bounded rank



$\text{Prob}(i_1, \ldots, i_p) =$
$\sum_{j=1}^{k} M^{(1)}_{i_1,j} \cdots M^{(p)}_{i_p,j}$

$v^{(q)}_j := M^{(q)}_{?,j} \in \mathbb{R}^n$
$\text{Prob} = \sum_{j=1}^{k} v^{(1)}_j \otimes \cdots \otimes v^{(p)}_j$

$\text{Model} = \{\text{tensors of rank} \leq k\}$
rank vs. *border rank*

Phylogenetic invariants

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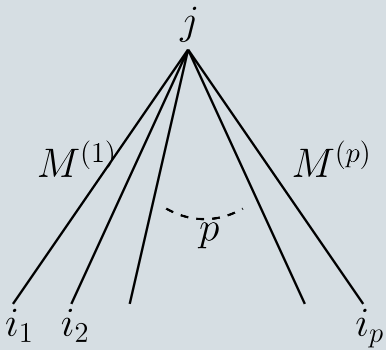

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rank vs. *border rank*

Equations for bounded rank

Classical

Ideal of $\{n \times n \times \cdots \times n$-tensors of rank $\leq 1\}$ is generated by 2×2-determinants.

Raicu, Landsberg-Manivel

Ideal of $\{n \times n \times \cdots \times n$-tensors of rank $\leq 2\}$ is generated by 3×3-determinants (*GSS conjecture*).

Strassen

Ideal of $\{3 \times 3 \times 3$-tensors of rank $\leq 4\}$ is generated by one polynomial of degree 9.

Friedland, Bates-Oeding

Equations for $4 \times 4 \times 4$-tensors of border rank ≤ 4.

Strassen's equation

$$
\begin{array}{c}
\mathbb{R}^3 \otimes \mathbb{R}^3 \otimes \mathbb{R}^3 \\
\Big\downarrow {\scriptstyle (x,y,z) \mapsto \begin{bmatrix} 0 & x & y \\ -x & 0 & z \\ -y & -z & 0 \end{bmatrix}} \\
\mathbb{R}^3 \otimes (\mathbb{R}^3 \otimes \mathbb{R}^3) \otimes \mathbb{R}^3 \\
\Big\downarrow \\
(\mathbb{R}^3 \otimes \mathbb{R}^3) \otimes (\mathbb{R}^3 \otimes \mathbb{R}^3) \\
\Big\downarrow \\
\mathbb{R}^9 \otimes \mathbb{R}^9
\end{array}
$$

maps rank 1 to rank 2
hence rank ≤ 4 to rank ≤ 8
take determinant!

Ottaviani-Landsberg
geometric interpretation
of Strassen-type equations

Equations for bounded rank

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Uniform degree bounds

Theorem (D-Kuttler)
For fixed k there exists a d s.t. $\forall p, n_1, \ldots, n_p$ the $n_1 \times \cdots \times n_p$-tensors of border rank $\leq k$ are defined by polynomials of degree $\leq d$.

d explicitly known only for $k = 1, 2$

Corollary
For fixed k there exists a polynomial-time probability-one algorithm for testing border rank $\leq k$.

Conjecture
Same statement for generators of the ideal.

Infinite-dimensional tensors

$V = \mathbb{R}^n$
$x_0, \ldots, x_{n-1} \in V^*$ coordinates
$V^{\otimes 1} \xleftarrow{I \otimes x_0} V^{\otimes 2} \xleftarrow{I \otimes I \otimes x_0} V^{\otimes 3} \longleftarrow \cdots$
$V^{\otimes \infty} := \lim_{\leftarrow} V^{\otimes p}$

coordinates $x_{i_1} \otimes x_{i_2} \otimes \ldots$
only finitely many i_j non-zero

$Y^\infty \subseteq V^{\otimes \infty}$ defined by vanishing of $(k+1) \times (k+1)$-determinants

Theorem
Y^∞ is Noetherian up to natural symmetries of $V^{\otimes \infty}$.

Very non-constructive??

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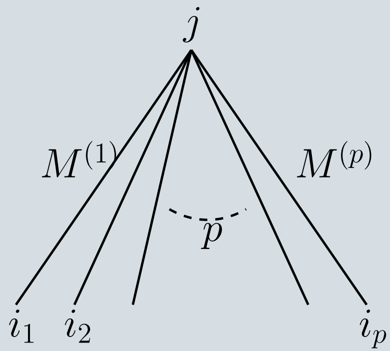


$\mathrm{Prob}(i_1, \ldots, i_p) = \sum_j M^{(1)}_{i_1,j} \cdots M^{(p)}_{i_p,j}$

now $i_1, \ldots, i_p, j \in G$ group

impose $M^{(q)}_{i,j} = m^{(q)}_{i-j}$

Sturmfels-Sullivant

Fourier transform:

$\widehat{\mathrm{Prob}}(i_1, \ldots, i_p) = \widehat{m}^{(1)}_{i_1} \cdots \widehat{m}^{(q)}_{i_q}$ if $i_1 + \ldots + i_q = 0$, and 0 else.

Degree bounds

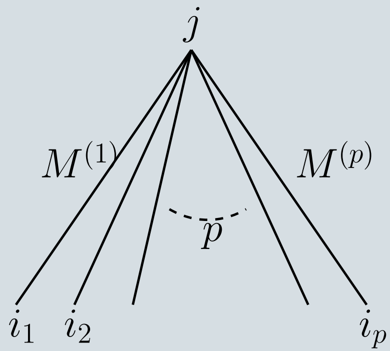
Conjecture (Sturmfels-Sullivant)
Ideal of $\text{Model}_{p,G}$ generated in degree $\leq |G|$ for all p.

proved by S-S for $G = C_2$
proved set-theoretically by Michalek for $G = C_2 \times C_2$ (3-Kimura model)

Infinite-dimensional approach
space with coordinates $x(i_1, i_2, \ldots)$
only finitely many i_j non-zero
and $i_1 + i_2 + \ldots = 0$
contains $\text{Model}_{\infty,G}$
large monoid of symmetries

Very near future
compute a finite *equivariant Gröbner basis* for $\text{Model}_{\infty,G}$
for $G = C_3, C_2 \times C_2, C_4, \ldots$

Group-based models



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Thank you!

Questions?