Tensors in Algebraic Statistics

Luis Sierra Muntané
luis.sierra@mail.utoronto.ca

Department of Statistical Sciences
University of Toronto

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Joint work with Marta Casanellas and Piotr Zwiernik.

Measures as tensors

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Tensors are multilinear maps that can be identified with m-way arrays. A *pure tensor* $e^1_{i_1} \otimes \cdots \otimes e^m_{i_m}$ acts as

$$\begin{aligned} \mathbb{R}^{r_1} \times \cdots \times \mathbb{R}^{r_m} &\longrightarrow \mathbb{R} \\ (e^1_{j_1}, \ldots, e^m_{j_m}) &\mapsto \begin{cases} 1 & \text{if } (j_1, \ldots, j_m) = (i_1, \ldots, i_m), \\ 0, & \text{otherwise} \end{cases} \end{aligned}$$

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For discrete r.v.s $X_i \in \mathcal{X}_i = \{0, \ldots, r_i - 1\}$, $i = 1, \ldots, m$
The p.m.f. $p = (p(x))_{x \in \mathcal{X}}$ of X can be then identified with a point

$$p(x) = \mathbb{P}(X_1 = x_1, \ldots, X_m = x_m) \in \mathbb{R}^{\mathcal{X}} := \bigotimes_{i=1}^{m} \mathbb{R}^{\mathcal{X}_i},$$

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whose projectivized space can be identified with the $m-1$ dimensional simplex

$$\Delta^{\mathcal{X}} \quad := \quad \{p \in \mathbb{R}^{\mathcal{X}} : \; p_x \geq 0, \sum_{x \in \mathcal{X}} p_x = 1\}.$$

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which correspond to semialgebraic constraints. As an example with two variables X_1, X_2:

$$p = p^1 \otimes p^2 = \begin{pmatrix} p^1_0 \\ \vdots \\ p^1_{r_1-1} \end{pmatrix} \begin{pmatrix} p^2_0 & \cdots & p^2_{r_2-1} \end{pmatrix}$$

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In the binary case $(X_1, X_2) \in \{0,1\}^2$. We have $\mu_{00} = p_{00} + p_{01} + p_{10} + p_{11} = 1$, $\mu_{10} = p_{10} + p_{11}$, $\mu_{01} = p_{01} + p_{11}$, $\mu_{11} = p_{11}$.

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$\implies$ Independence model is given by $\kappa_{11} = 0$. For the study of binary cumulant varieties see (Sturmfels and Zwiernik, 2013).

Remark (Absolutely continuous measures)

The absolutely continuous case is also possible, where the moment tensors are *symmetric* (McCullagh, 2018):

$$\mu_{i_1 \dots i_r}(X) = \mathbb{E} X_{i_1} \cdots X_{i_r} = \frac{\partial^r}{\partial s_{i_1} \cdots \partial s_{i_r}} M_X(\mathbf{s}) \Big|_{\mathbf{s}=0} \,,$$

$$\kappa_{i_1 \dots i_r}(X) \;=\; \mathrm{cum}(X_{i_1}, \dots, X_{i_r}) \;=\; \frac{\partial^r}{\partial s_{i_1} \cdots \partial s_{i_r}} \log M_X(\mathbf{s}) \Big|_{\mathbf{s}=0} \,.$$

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Useful for multivariate Gaussian models $\mathcal{N}_m(\mu,\Sigma)$, where conditional independences correspond to linear restrictions $\left(\Sigma^{-1}\right)_{ij} = 0$ (Uhler, 2017).

Tensor rank

An $n_1 \times n_2$ matrix has rank $\leq k$ if

$$M = u^1 \otimes v^1 + \cdots + u^k \otimes v^k, \quad \text{for } u^i \in \mathbb{R}^{n_1},\, v^i \in \mathbb{R}^{n_2}.$$

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Finding such a decomposition is `NP`-hard! (Hillar and Lim, 2013)

Naive Bayes

Consider the m-variate the dataset $\{(X_1, \ldots, X_m)\}$ with $X_i \in \mathcal{X}_i = [r_i]$, where each point belongs to the class $H \in \mathcal{C} = [k]$.

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$$X_i \perp\!\!\!\perp X_j \mid H, \quad \forall i, j \in [m]$$

$$\mathbb{P}(H = h \mid X = x) \propto p(h) \prod_{i=1}^{m} \mathbb{P}(X_i = x_i \mid H = h)$$

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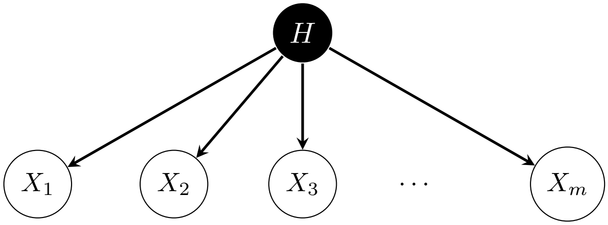

Naive Bayes II

Since the X_i are discrete, we can encode the conditionals as

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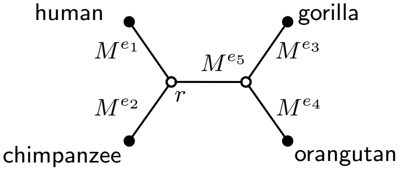
and then the marginal over the observables is naturally given as a tensor

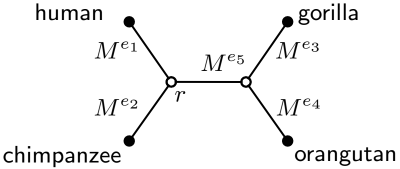
$$\mathbb{P}(X = x) = \sum_{h \in \mathcal{C}} p(h) \cdot u^{1,h} \otimes \cdots \otimes u^{m,h},$$

whose nonnegative rank is therefore no larger than k.



Consider species as vertices of a directed tree $\mathcal{T} = (V, E)$, $m = |L|$ leaves, $\deg(v) > 2$ for $u \in V \setminus L$, with nucleotides $X_u = \{\mathtt{A}, \mathtt{C}, \mathtt{G}, \mathtt{T}\}$.

Phylogenetic Trees



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$$\begin{array}{c}\mathtt{ACGTGACTGATCAGCTGACT} \\ \Big\downarrow M^e \\ \mathtt{ACGTTACTGATCAGCTGACT}\end{array}$$

$M^e_{x,y} = \mathbb{P}(X_v = y \,|\, X_u = x)$ are transition matrices for $e = \{u \to v\}$.

Phylogenetic Trees II

$$\mathbb{P}\left(\{x_v\}_{v\in V}\right) = \mathbb{P}(x_r) \prod_{e=\{u\to w\}\in E} M^e_{x_w,x_u},$$

since all interior nodes are latent, and marginalizing over them realizes a tensor

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so that the leaf nucleotides follow the distribution

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Now consider a split of the leaves $L = A \sqcup B$

$$\begin{array}{rcl} \mathbb{R}^{\mathcal{X}} \cong \mathbb{R}^{\mathcal{X}_A} \otimes \mathbb{R}^{\mathcal{X}_B} & \longrightarrow & \mathcal{M}_{|\mathcal{X}_A|\times|\mathcal{X}_B|}(\mathbb{R}) \\ p = (p_{x_1\dots x_n}) & \mapsto & \mathrm{flatt}_{A|B}(p), \end{array}$$

where the matrix $\mathrm{flatt}_{A|B}(p)$ has entries $\mathbb{P}(X_A = x_A, X_B = x_B)$.

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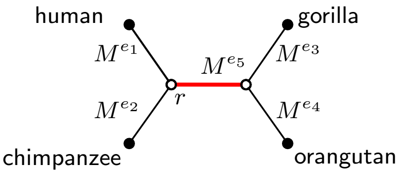

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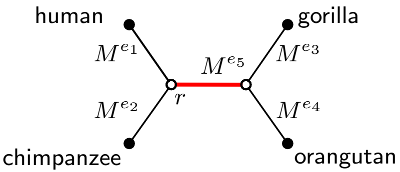

Denoting $L = \{\text{human, chimpanzee, gorilla, orangutan}\}$ by $\{1, 2, 3, 4\}$, the flattened tensor is given by

$$\text{flatt}_{12|34}(p) = \begin{pmatrix} p_{0000} & p_{0001} & p_{0002} & \cdots & p_{0033} \\ p_{0100} & p_{0101} & p_{0102} & \cdots & p_{0133} \\ p_{0200} & p_{0201} & p_{0202} & \cdots & p_{0233} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ p_{3300} & p_{3301} & p_{3302} & \cdots & p_{3333} \end{pmatrix}.$$

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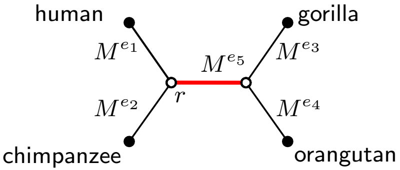

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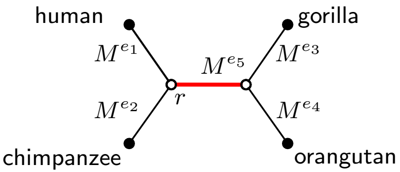

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$\implies$ $p_{\mathcal{T}}$ has (nonnegative) rank at most 4,

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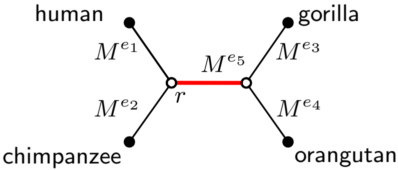

Denoting $L = \{\text{human, chimpanzee, gorilla, orangutan}\}$ by $\{1, 2, 3, 4\}$, the flattened tensor is given by

$$\mathrm{flatt}_{12|34}(p) = \begin{pmatrix} p_{0000} & p_{0001} & p_{0002} & \cdots & p_{0033} \\ p_{0100} & p_{0101} & p_{0102} & \cdots & p_{0133} \\ p_{0200} & p_{0201} & p_{0202} & \cdots & p_{0233} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ p_{3300} & p_{3301} & p_{3302} & \cdots & p_{3333} \end{pmatrix}.$$

$\Longrightarrow$ This is a Naive Bayes model with $m = 2$,

$\Longrightarrow$ $p_{\mathcal{T}}$ has (nonnegative) rank at most 4,

$\Longrightarrow$ $\mathrm{flatt}_{A|B}(p_{\mathcal{T}})$ has matrix rank at most 4.

Phylogenetic Trees III

Theorem (Allman and Rhodes (2008))

For $\mathcal{T}$ a phylogenetic tree and $A|B$ a split of its leaves L, let $p_{\mathcal{T}}$ be the tensor distribution obtained from a Markov process on $\mathcal{T}$. Then, assuming some genericity conditions

1. *If $A|B$ is an edge split, $\mathrm{flatt}_{A|B}(p_{\mathcal{T}})$ has rank less than or equal to 4.*
2. *If $A|B$ is not an edge split, the rank of $\mathrm{flatt}_{A|B}(p_{\mathcal{T}})$ is larger than 4*

Identifiability of tensor models (Allman et al., 2009), applications to genomic reconstruction (Fernández-Sánchez and Casanellas, 2016).

Mixture Models

From a family of distributions $\mathcal{P}$ we can construct the mixture model

$$\mathrm{Mixt}^k\left(\mathcal{P}\right) = \left\{ \sum_{i=1}^{k} \pi_i p^i \;:\; \pi \in \Delta^{k-1},\, p^i \in \mathcal{P} \right\}.$$

Upon taking the Zariski closure, mixtures models in statistics correspond to join varieties and secant varieties in algebraic geometry.

Examples: Gaussian mixtures, topic models, Latent Dirichlet Allocation (LDA) etc.

Model fitting: EM algorithm Dempster et al. (1977).

Challenges and Remarks

- The Best Low-Rank Approximation Problem is ill-posed.
- Most Tensor problems are NP-hard Hillar and Lim (2013).
- Average case polynomial-time heuristics being developed.
- `algstat` R package for algebraic statistics.
- Alpha tensor by Google DeepMind for tensor decompositions.

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