# ALGEBRAIC STATISTICS AND CONTINGENCY TABLES

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AML08: Algebraic Methods in Machine Learning Symposium and Workshop at NIPS'08

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# Some Revelant Publications

- Dobra, A. and Fienberg, S.E. (2000). Bounds for cell entries in contingency tables given marginal totals and decomposable graphs. PNAS, 97(22), 1185–11892.
- Obbra, A., Karr, A.F. and Sanil, A.P. (2003). Preserving confidentiality of high-dimensional tabulated data: statistical and computational issues. Statistics and Computing, 13, 363–370.
- Dobra, A. (2003). Markov bases for decomposable graphical models. Bernoulli, 9(6), 1093–1108.
- Dobra, A. and Sullivant, S. (2004). A divide-and-conquer algorithm for generating Markov bases for multi-way tables. Computational Statistics, 19, 347–366.
- Dobra, A., Tebaldi, C. and West, M. (2006). Data augmentation in multi-way contingency tables with fixed marginal totals. JSPI, 136, 355–372.

### Only 810 tables consistent with marginals $\mathcal{R}_1!!$ .

 $\mathcal{R}_1 = \left\{ [\textit{ACDEF}], [\textit{ABDEF}], [\textit{ABCDE}], [\textit{BCDF}], [\textit{ABCF}], [\textit{BCEF}] \right\}.$ 

				B	B no		yes		В	no		yes	
F	Е	D	С	A	no	yes	no	yes	A	no	yes	no	yes
neg	< 3	< 140	no		44	40	112	67		[35, 45]	[35, 44]	[111, 121]	[63, 72]
			yes		129	145	12	23		[128, 138]	[141, 150]	[3, 13]	[18, 27]
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TABLE: Czeck Autoworkers data from Edwards & Havranek (1985) (left panel) and bounds given marginals  $\mathcal{R}_1$  (right panel).



### How to do inference under log-linear models $A_1$ - $A_8$ ?

Log-linear Model	Minimal Sufficient Statistics
$\mathcal{A}_1$	$\mathcal{R}_1 \cup \{[BCDEF]\}$
$\mathcal{A}_2$	$\mathcal{R}_1 \cup \{[ABCEF]\}$
$\mathcal{A}_3$	$\mathcal{R}_1 \cup \{[ABCDF]\}$
$\mathcal{A}_4$	$\mathcal{R}_1 \cup \{[BCDEF], [ABCEF]\}$
$\mathcal{A}_5$	$\mathcal{R}_1 \cup \{[BCDEF], [ABCDF]\}$
$\mathcal{A}_6$	$\mathcal{R}_1 \cup \{[ABCEF], [ABCDF]\}$
$\mathcal{A}_7$	$\mathcal{R}_1 \cup \{[BCDEF], [ABCEF], [ABCDF]\}$
$\mathcal{A}_{8}$	Saturated



# Multi-way Tables with Fixed Marginals Notation & Relevant issues

 $\mathcal{K} = \{1, 2, \dots, k\}, \ \mathbf{X} = (X_1, X_2, \dots, X_k) \text{ cross-classified in } \mathbf{n} = \{n(i)\}_{i \in \mathcal{I}}.$  $\mathcal{I} = \mathcal{I}_1 \times \mathcal{I}_2 \times \dots \times \mathcal{I}_k, \ \mathcal{I}_j = \{1, 2, \dots, l_j\}, \ l_j \in \{1, 2, \dots\}.$ 

Tables consistent with fixed marginals:

$$T(\mathbf{n}_{D_1},\ldots,\mathbf{n}_{D_r})=\{\mathbf{x}=\{x(i)\}_{i\in\mathcal{I}}:\mathbf{x}_{D_1}=\mathbf{n}_{D_1},\ldots,\mathbf{x}_{D_r}=\mathbf{n}_{D_r}\}.$$

#### Questions of interest

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 $\min\{\pm x(i): i \in \mathcal{I}, \mathbf{x} \in T(\mathbf{n}_{D_1}, \ldots, \mathbf{n}_{D_r})\}.$ 

- 2 Enumerate tables in  $T(\mathbf{n}_{D_1}, \ldots, \mathbf{n}_{D_r})$ .
- **3** Estimate size of  $T(\mathbf{n}_{D_1}, \ldots, \mathbf{n}_{D_r})$ .
- Sample from  $T(\mathbf{n}_{D_1},\ldots,\mathbf{n}_{D_r})$ .
- Probability distributions on  $T(\mathbf{n}_{D_1}, \ldots, \mathbf{n}_{D_r})$ .

- G = (K, E) associated with  $\mathbf{n}_{D_1}, \dots, \mathbf{n}_{D_r}$  has edges:  $E = \{(u, v) : \{u, v\} \subset D_j \text{ for some } j\}.$
- Interpretation: if  $(u, v) \notin E$ , then

$$X_u \bot X_v | X_{K \setminus \{u,v\}} \Leftrightarrow u \bot v | K \setminus \{u,v\}.$$

- Special types of graphs:
  - decomposable,
  - 2 reducible.



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#### SPECIAL TYPES OF GRAPHS Decomposable independence graphs

- $D_1 = \{1, 3, 4, 11\}, D_2 = \{3, 4, 7, 8, 9, 11\}, D_3 = \{2, 3, 9, 10\}, D_4 = \{4, 5, 6, 7\}.$
- $S_1 = \{3, 4, 11\}, S_2 = \{3, 9\}, S_3 = \{4, 7\}.$
- Fixed marginals:  $\mathbf{n}_{D_1}$ ,  $\mathbf{n}_{D_2}$ ,  $\mathbf{n}_{D_3}$ ,  $\mathbf{n}_{D_4}$ .
- Cliques:  $C(G) = \{D_1, D_2, D_3, D_4\}$ ; Separators:  $S(G) = \{S_1, S_2, S_3\}$ .



#### Theorem

[Dobra & Fienberg, 2000] Let G = (K, E) decomposable. Let C(G) be the cliques of G and S(G) the separators of G. Then:

$$\min \left\{ n_{\mathcal{C}}(i_{\mathcal{C}}) | \mathcal{C} \in \mathcal{C}(\mathcal{G}) \right\} \ge n(i) \ge \\ \max \left\{ \sum_{\mathcal{C} \in \mathcal{C}(\mathcal{G})} n_{\mathcal{C}}(i_{\mathcal{C}}) - \sum_{\mathcal{S} \in \mathcal{S}(\mathcal{G})} n_{\mathcal{S}}(i_{\mathcal{S}}), 0 \right\}$$

Example:

$$\min \{n_{D_1}, n_{D_2}, n_{D_3}, n_{D_4}\} \ge n(i) \ge \\ \max \{n_{D_1} + n_{D_2} + n_{D_3} + n_{D_4} - n_{S_1} - n_{S_2} - n_{S_3}, 0\}.$$



# SPECIAL TYPES OF UNDIRECTED GRAPHS REDUCIBLE INDEPENDENCE GRAPHS

- $D_1 = \{1, 3, 4, 11\}, D_2 = \{3, 4, 7, 8, 9, 11\}, D_3 = \{2, 3, 9, 10\}, D_4 = \{4, 5, 6, 7\}.$
- $S_1 = \{3, 4, 11\}, S_2 = \{3, 9\}, S_3 = \{4, 7\}.$
- Fixed marginals:  $\mathbf{n}_{S_1}$  and all two-way marginals given by edges!!
- Prime components:  $C(G) = \{D_1, D_2, D_3, D_4\}$ ; Separators:  $S(G) = \{S_1, S_2, S_3\}$ .



#### Theorem

[Dobra & Fienberg, 2000] Let G = (K, E) reducible. Let C(G) be the prime components of G and S(G) the separators of G. Then:

$$\min\left\{n_{C}^{U}(i_{C})|C \in C(G)\right\} \ge n(i) \ge \\ \max\left\{\sum_{C \in C(G)} n_{C}^{L}(i_{C}) - \sum_{S \in S(G)} n_{S}(i_{S}), 0\right\}.$$

### Example:

$$\min \{ n_{D_1}^U, n_{D_2}^U, n_{D_3}^U, n_{D_4}^U \} \ge n(i) \ge \\ \max \{ n_{D_1}^L + n_{D_2}^L + n_{D_3}^L + n_{D_4}^L - n_{S_1} - n_{S_2} - n_{S_3}, 0 \}.$$



- Generalized version of the Shuttle Algorithm (Buzzigoli & Giusti).
- Exploit the tree-like structure of the problem.
- $\bullet \ \mathcal{C}$  cells obtained by collapsing across categories.
- New formulation of the bounds problem:
   Find the bounds C<sup>U</sup> and C<sup>L</sup> for the cells C given information about some cells C<sub>0</sub> ⊂ C.
- Let  $c_1, c_2 \in \mathcal{C}$  such that their join  $c_{12}$  is still in  $\mathcal{C}$ . Then:

$$\begin{split} c_1^L + c_2^L &\leq c_{12} \leq c_1^U + c_2^U, \\ c_{12}^L - c_2^U &\leq c_1 \leq c_{12}^U - c_2^L. \end{split}$$

Example:  $2 \times 3$  table with fixed row and column totals.



**Example**: There is no  $6 \times 4 \times 3$  integer table having the two-way margins (Vlach, 1986):



**Example**: There are only two  $3 \times 4 \times 6$  tables with marginals:

$$n_{12} = \begin{pmatrix} 2 & 2 & 2 & 2 \\ 3 & 1 & 1 & 1 \\ 2 & 2 & 2 & 2 \end{pmatrix}, n_{13} = \begin{pmatrix} 2 & 1 & 2 & 3 & 0 & 0 \\ 2 & 1 & 0 & 0 & 2 & 1 \\ 0 & 0 & 2 & 1 & 2 & 3 \end{pmatrix},$$
$$n_{23} = \begin{pmatrix} 2 & 1 & 2 & 0 & 2 & 0 \\ 1 & 0 & 2 & 0 & 0 & 2 \\ 1 & 0 & 0 & 2 & 2 & 0 \\ 0 & 1 & 0 & 2 & 0 & 2 \end{pmatrix}.$$

Possible values for cell (1, 1, 1) are 0 and 2!!



Example: 2<sup>16</sup> table with three fixed 15-way marginals:

- 62,384 zero entries out of  $2^{16} = 65,536$  cells.
- Only 128 cells have upper bounds strictly bigger than lower bounds.
- 1,729 (499) cells have counts of 1 (2).
- 1,698 (485) of these cells have upper bounds equal lower bounds.



## How to produce a full table consistent with a set of fixed marginals?

- Global moves
  - Generated from the Generalized Shuttle Algorithm.
  - Could take a long time to compute.
  - Can balance between "long" and "short" jumps.
  - $\bullet\,$  Can be used to estimate # of tables consistent with fixed marginals.
- 2 Local moves (Markov bases)
  - Formulas for decomposable case (Dobra, 2003).
  - Otherwise, need algebraic methods (Groebner bases).
  - Very fast once available!



- Order the cells in table:  $\mathcal{I} = \{i^1, i^2, \dots, i^m\}.$
- Possible current values for cell *i*<sup>a</sup>:

$$\mathcal{H}_a := \{L(i^a), L(i^a) + 1, \dots, U(i^a) - 1, U(i^a)\}.$$

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- Choose scaling factors  $v_a \in (0,1)$ ,  $a = 1, \ldots, m$ .
- Generate a candidate table **n**\* as follows:

end for

#### IMPUTING CELL COUNTS Estimating number of feasible table using global moves

 $\mathcal{M}(T)$  is number of tables in  $T = T(\mathbf{n}_{D_1}, \dots, \mathbf{n}_{D_r})$ . Assume uniform distribution on T:

$$p(\mathbf{n}) = \frac{1}{\mathcal{M}(\mathcal{T})}.$$

Set scaling factors  $v_a$  equal to one:

$$q(n) \propto \prod_{a=1}^m \frac{1}{U(i^a)-L(i^a)+1}.$$

Write:

$$1 = \sum_{\mathbf{n}\in T} \frac{p(\mathbf{n})}{q(\mathbf{n})} q(\mathbf{n}) \Rightarrow \mathcal{M}(T) = \sum_{\mathbf{n}\in T} \frac{1}{q(\mathbf{n})} q(\mathbf{n}).$$

Estimate  $\hat{\mathcal{M}}(T) = \frac{1}{S} \sum_{s=1}^{S} \frac{1}{q(\mathbf{n}^{(S)})}$  where  $\mathbf{n}^{(1)}, \dots, \mathbf{n}^{(S)}$  independently sampled from  $q(\cdot)$ .

 $\mathcal{R}_2$  are the 15 four-way marginals.  $\mathcal{R}_3 = \{[BF], [ABCE], [ADE]\}$ 

В no yes В no yes С А А F D E no yes no ves no ves no yes < 3 < 140 [27, 58][25, 56][96, 134][44, 82][0, 88][0, 62][0, 224][0, 117]neg no [108, 149][123, 168] [0, 22][9, 37] [0, 261][0, 246][0, 24][0, 38]yes > 140[22, 49] [0, 24][60, 96] [16, 52][0, 88][0, 62][0, 224][0, 117]no [91, 127][45,85] [0, 18][0, 20][0, 261][0, 151][0, 24][0, 38]yes > 3 < 140 [10, 37] [17, 44][48, 86] [49, 89] [0, 58][0, 60][0, 170][0, 148] no [0, 173][0, 20]yes [30, 68][58, 102] [0, 19][0, 25][0, 115][0, 36]> 140[13, 37] [8, 36] [55, 90] [38, 76] [0, 58][0, 60][0, 170][0, 148]no [30, 67] [45, 86] [0, 19][0, 27] [0, 115][0, 173][0, 36] [0, 20]yes < 3 pos < 140 [0, 15][0, 13][4, 31][0, 23][0, 88][0, 62][0, 125][0, 117]no [0, 21][3, 30] [0, 10][0, 9] [0, 134][0, 134][0, 10][0, 38]yes > 140[0, 11][0, 10][0, 24][0, 18][0, 88][0, 62][0, 125][0, 117]no 0, 26 [2, 30] [0, 11][0, 9][0, 134][0, 134][0, 24] [0, 38] yes > 3 < 140 [1, 14][0, 9][0, 26][0, 26][0.58] [0, 60][0, 125][0, 125]no [0, 19][4, 29][0, 9][0, 9][0, 115][0, 134][0, 20][0, 36]yes  $\geq$  140 [0, 9][0, 9] [0, 22][0, 58][0, 60][0, 125][0, 125]no [0, 26][0, 19][0, 23][0, 9][0, 13][0, 115][0, 134][0, 20][0, 36] yes

TABLE: Bounds given  $\mathcal{R}_2$  (left-hand panel) and  $\mathcal{R}_3$  (right-hand panel).

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 $\mathcal{R}_2$  are the 15 four-way marginals. 705,884 tables consistent with  $\mathcal{R}_2$ . Estimated number of tables: 703,126. 95% CI is 650,000–750,000.

 $\begin{aligned} \mathcal{R}_3 &= \{[BF], [ABCE], [ADE]\}. \\ \text{Estimated number of tables consistent with } \mathcal{R}_3: \ 10^{58}. \\ 95\% \ \text{Cl is} \ 10^{57} \text{--} 10^{59}. \end{aligned}$ 



### DEFINITION

A local move  $\mathbf{g} = \{g(i)\}_{i \in \mathcal{I}}$  is a multi-way array with integer entries  $g(i) \in \{\dots, -2, -1, 0, 1, 2, \dots\}$ .

#### DEFINITION

A Markov basis for  $T = T(\mathbf{n}_{D_1}, \dots, \mathbf{n}_{D_r})$  allows any two tables  $\mathbf{n}_1$ ,  $\mathbf{n}_2$  in T to be connected by a series of local moves:

$$\mathbf{n}_1 - \mathbf{n}_2 = \sum_{j=1}^r \mathbf{g}^j.$$



Primitive moves for  $2x^2$  tables:

<i>n</i> +1	<i>n</i> <sub>+2</sub>	n <sub>++</sub>
$n_{21} - 1$	$n_{22} + 1$	n <sub>2+</sub>
$n_{11} + 1$	$n_{12} - 1$	<i>n</i> <sub>1+</sub>

Primitive moves for two-way tables:

$$g^{i_1i_2;j_1j_2}(i,j) = \begin{cases} 1, & \text{if } (i,j) \in \{(i_1,j_1), (i_2,j_2)\}.\\ -1, & \text{if } (i,j) \in \{(i_1,j_2), (i_1,j_2)\},\\ 0, & \text{otherwise.} \end{cases}$$

Extension to decomposable models with two cliques!!

#### Theorem

[Dobra, 2001] A well defined set of primitive moves connects all tables having a set of fixed marginals  $\mathbf{n}_{D_1}, \ldots, \mathbf{n}_{D_r}$ , when this set of marginals are the cliques  $\{D_1, \ldots, D_r\}$  of a decomposable graph G = (K, E).

#### Proof.

For every separator  $S_j$  of G there exists a proper decomposition of G:  $(V_j^1 \setminus S_j, S_j, V_j^2 \setminus S_j)$ . A Markov basis for  $D_1, \ldots, D_r$  is:

$$\mathsf{MB}(D_1,\ldots,D_r)=\bigcup_{j=2}^r\mathsf{F}(V_j^1,V_2^j).$$

Divide-and-conquer technique to generate Markov bases for reducible graphs!!



### IMPUTING CELL COUNTS Example: Markov bases for decomposable graphical models

- $D_1 = \{1, 3, 4, 11\}, D_2 = \{3, 4, 7, 8, 9, 11\}, D_3 = \{2, 3, 9, 10\}, D_4 = \{4, 5, 6, 7\}.$
- $S_1 = \{3, 4, 11\}, S_2 = \{3, 9\}, S_3 = \{4, 7\}.$
- $MB(D_1, D_2, D_3, D_4) = F(D_1, \{2, \dots, 11\}) \cup F(D_2, \{1, 3, \dots, 9, 11\}) \cup F(D_4, \{1, \dots, 4, 7, \dots, 11\}).$



# PROBABILITY DISTRIBUTIONS ON SPACES OF TABLES NOTATIONS

- $\mathbf{n} = \{n(i)\}_{i \in \mathcal{I}}$  multi-way table.
- $\mathcal{D}$  is available data (e.g., marginals, bounds, structural zeros).
- $\mathcal{T}$  tables consistent with  $\mathcal{D}$ .
- Cell counts  $n(i) \sim Poisson(\lambda(i)), \lambda(i) > 0.$

$$p(\mathcal{D}|\lambda) = \sum_{\mathbf{n}' \in \mathcal{T}} p(\mathbf{n}'|\lambda).$$
  

$$p(\mathbf{n}, \mathcal{D}|\lambda) = p(\mathbf{n}|\lambda) \cdot I_{\{\mathbf{n} \in \mathcal{T}\}}.$$
  

$$p(\mathbf{n}|\mathcal{D}, \lambda) = \frac{p(\mathbf{n}|\lambda)}{p(\mathcal{D}|\lambda)} \cdot I_{\{\mathbf{n} \in \mathcal{T}\}}.$$

# PROBABILITY DISTRIBUTIONS ON SPACES OF TABLES LOG-LINEAR MODELS FOR POISSON MEANS

Let  $\mathcal{A}$  log-linear model for  $\lambda = \{\lambda(i)\}_{i \in \mathcal{I}}$ :

$$\lambda(i) = \mu \prod_{C} \psi_{C}(i_{C}).$$

#### Theorem

If marginal  $\mathbf{n}_{C}$  determined from  $\mathcal{D}$ , then, under  $\mathcal{A}$ ,  $p(\mathbf{n}|\mathcal{D}, \lambda)$  does not depend on  $\psi_{C}(i_{C})$ .

### Theorem

The hypergeometric distribution is obtained by conditioning on a log-linear model whose parameters are determined from  $\mathcal{D}$ .



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$\mathcal{A}_{8}$	Saturated



Let  $\mathcal{A}$  log-linear model with parameters  $\theta$  for Poisson means  $\lambda$ .

At the *s*-th step of algorithm do:

- Simulate  $\theta^{(s+1)}$  from  $p(\theta|\mathcal{A}, \mathbf{n}^{(s)}) \propto p(\theta|\mathcal{A})p(\mathbf{n}^{(s)}|\lambda(\theta))$ . Compute  $\lambda^{(s+1)} = \lambda(\theta^{(s+1)})$ .
- ② Simulate  $\mathbf{n}^{(s+1)}$  from  $p(\mathbf{n}|\mathcal{D}, \lambda^{(s+1)})$ .

Independent Gamma (Uniform) priors for  $\lambda$  imply conjugate (truncated) Gamma posteriors (West, 1997; Tebaldi & West (1998)).



# EXAMPLE: CZECH AUTOWORKERS DATA AUGMENTATION



FIGURE: Convergence of the data augmentation method for the Czech autoworkers data. The x-axis represents the iteration number on a  $\log_{10}$  scale, while the y-axis gives the sample mean of  $\lambda_0$  from five starting points under model  $\mathcal{A}_8$ .

# EXAMPLE: CZECH AUTOWORKERS DATA AUGMENTATION



FIGURE: Approximate posterior distributions for  $\lambda_0$  under the log-linear models  $\mathcal{A}_1, \ldots, \mathcal{A}_8$ . The dotted lines represent estimates of the posterior mode and the corresponding 95% confidence intervals.



- (I) Computing exact p-values.
- $({\rm II})\,$  Methods for sparse tables.

