

# Maximum Likelihood Estimation in Loglinear Models

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April 18, 2012  
Workshop on Graphical Models:  
Mathematics, Statistics and Computer Sciences

Fields Institute

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- The MLE may not exist due to **sampling zeros**.
- Nonexistence of the MLE largely ignored in practice. Important issue, particular in large and sparse tables.

## Motivating Pathological Example

- Consider a  $2^3$  table and the model  $[12][13][23]$


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- Zero margin: MLE does not exist!

0	1	2	3
0	4	2	2

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- Haberman's example (1974). Positive margins and nonexistent MLE.

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- Always perfect fit to the data. The p-value is always 1.

# Outline

- Background on log-linear models and exponential families.
- Existence of the MLE.
- Parameter estimability under a nonexistent MLE.
- Computation of extended MLE.

# Log-Linear Models

- Consider the exponential family  $\{P_\theta, \theta \in \mathbb{R}^{\mathcal{I}}\}$  over a finite set of *cells*  $\mathcal{I}$ :

$$P_\theta(\{i\}) = \exp\{(\theta, \mathbf{a}_i) - \phi(\theta)\}, \quad \theta \in \mathbb{R}^d, i \in \mathcal{I},$$

with  $\mathbf{a}_i \in \mathbb{N}^d \setminus \{0\}$  and  $\phi(\theta) = \log(\sum_i \exp\{(\theta, \mathbf{a}_i)\})$ .

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- Observe a number  $N$  (possibly random) of cells  $\{L_1, \dots, L_N\}$ , with  $L_j \in \mathcal{I}$ , all  $j$ .

The corresponding **contingency table** is the random vector  $n \in \mathbb{N}^{\mathcal{I}}$

$$n(i) = |\{j: L_j = i\}|, \quad i \in \mathcal{I}.$$

# Log-Linear Models

- Log-linear model analysis (see, e.g. Haberman, 1974 and Bishop et al., 2007) is concerned with modeling the distribution of  $n$  by assuming that
  - $m := \mathbb{E}(n) > 0$ ,
  - $\mu := \log(m) \in \mathcal{M} \subset \mathbb{R}^{\mathcal{I}}$ , where  $\mathcal{M} = \mathcal{R}(A)$  is the **log-linear subspace**.
- **Sampling constraints:** let  $\mathcal{N} \subset \mathcal{M}$  be a linear subspace of  $\mathcal{M}$  of dimension  $m < d$ : **sampling subspace**.

**Conditional Poisson sampling:**  $\{n(i), i \in \mathcal{I}\}$  have the conditional distribution of  $|\mathcal{I}|$  independent Poisson random variables with means  $\{\exp(\mu(i)), i \in \mathcal{I}\}$  given that  $\Pi_{\mathcal{N}} n = c$  for some known  $c \in \mathbb{R}^{\mathcal{I}}$ .

## Conditional Poisson Sampling Schemes: Examples

- **Poisson Likelihood:**  $\mathcal{N} = \{0\}$ . The log-likelihood is

$$(n, \mu) - \sum_i \exp(\mu(i)) - \sum_i \log(n(i))!, \quad \mu \in \mathcal{M}.$$

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- **Product Multinomial Likelihood:**  $\mathcal{N} = \text{span}(\chi_1, \dots, \chi_m)$ , where the  $\chi_j$ 's are the indicator functions of a partition of  $\mathcal{I}$ . The sampling constrains are  $(n, \chi_j) = N_j > 0$  for all  $j$ .

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- **Poisson-Multinomial likelihood (Lang, 2005):** a combination of the two.

## Example: Hierarchical Log-Linear Models

- Let  $X_1, \dots, X_K$  be discrete random variables, each  $X_k$  supported on finite set  $\mathcal{I}_k$  of labels. Then  $\mathcal{I} = \times_{k=1}^K \mathcal{I}_k$ .  
 A **hierarchical log-linear model**  $\Delta$  is a simplicial complex: class of subsets of  $\{1, \dots, K\}$  such that  $S \in \Delta$  and  $T \subset S$  implies  $T \in \Delta$ .  
**Graphical models** are special cases.
- There log-linear subspaces are of ANOVA-type and there are canonical ways of constructing  $\Delta$  (see Lauritzen, 1996, Appendix B).

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**Graphical models** are special cases.
- There log-linear subspaces are of ANOVA-type and there are canonical ways of constructing  $\Lambda$  (see Lauritzen, 1996, Appendix B).
- Inferential tasks: estimation, goodness-of-fit testing and model selection.**

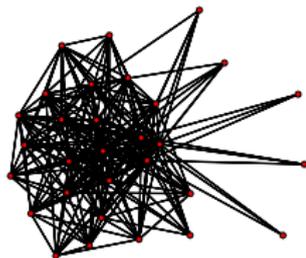
## Example: Hierarchical Log-Linear Models

Mildew fungus example:  $2^6$  sparse table. Source: Edwards (2000).

			1		2				D		
			1		2		1		2		E
			1	2	1	2	1	2	1	2	F
1	1	1	0	0	0	0	3	0	1	0	
		2	0	1	0	0	0	1	0	0	
	2	1	1	0	1	0	7	1	4	0	
		2	0	0	0	2	1	3	0	11	
2	1	1	16	1	4	0	1	0	0	0	
		2	1	4	1	4	0	0	0	0	1
	2	1	0	0	0	0	0	0	0	0	
		2	0	0	0	0	0	0	0	0	
A	B	C									

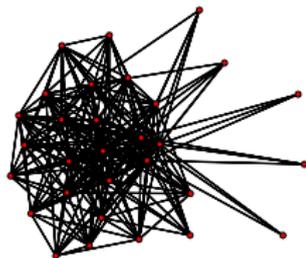
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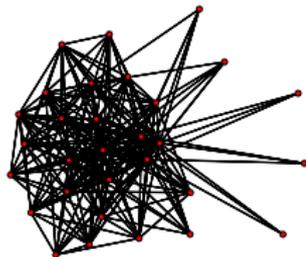


- $\beta$ -Model**: edges are independent and occurs with probabilities

$$\frac{e^{\beta_i + \beta_j}}{1 + e^{\beta_i + \beta_j}}, \quad i \neq j, \quad \beta = (\beta_1, \dots, \beta_v) \in \mathbb{R}^v.$$

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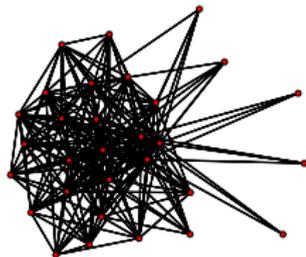
The probability of a graph  $x \in \mathcal{G}_n$  is

$$\exp \left\{ \sum_{i=1}^v d_i \beta_i - \psi(\beta) \right\}, \quad \beta \in \mathbb{R}^v,$$

where  $d(x) = d = (d_1, \dots, d_v)$  is the (ordered) degree sequence of  $x$ .

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- It is a log-linear model under product multinomial sampling.

# Exponential Family Representation

- It is more convenient to represent the log-linear model likelihood in exponential form, with densities

$$p_{\theta}(n) = \exp \left\{ (\mathbf{A}^{\top} n, \theta) - \psi(\theta) \right\} \nu(n), \quad \theta \in \mathbb{R}^d,$$

where  $n \in \mathcal{S}(\mathcal{N}, \mathbf{c}) := \{x \in \mathbb{N}^{\mathcal{I}} : \Pi_{\mathcal{N}} x = \mathbf{c}\}$  and the base measure is

$$\nu(x) = 1_{x \in \mathcal{S}(\mathcal{N}, \mathbf{c})} \prod_{i \in \mathcal{I}} \frac{1}{x(i)!}, \quad x \in \mathbb{N}^{\mathcal{I}}.$$

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- It is a family of order  $d - m$ , where  $m = \dim(\mathcal{N}) > 0$ . Minimality: replace  $\mathbf{A}$  with full-rank  $\mathbf{A}'$  such that  $\mathcal{R}(\mathbf{A}') = \mathcal{M} \ominus \mathcal{N} := \mathcal{M} \cap \mathcal{N}^c$ .

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- Better log-likelihood model parametrization for product-multinomial sampling:

$$(n, \beta) - \sum_{j=1}^m N_j \log(\exp^{\beta}, \chi_j) - \sum_{i \in \mathcal{I}} \log n(i)!, \quad \beta \in \mathcal{M} \ominus \mathcal{N}.$$

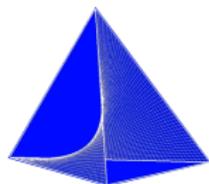
## Three views of Log-Linear Models

- 1 The exponential family natural parametrization:  $\mathbb{R}^{d-m}$ .
- 2 The log-linear model parametrization:  $\mathcal{M} \ominus \mathcal{N} \subset \mathbb{R}^{\mathcal{I}}$ .

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- 3 **Connection with Algebraic Geometry** (see, e.g., Drton et al. 2008).  
 Let  $M = \{\exp^\mu, \mu \in \mathcal{M}\}$ : intersection of a real toric variety in  $\mathbb{R}^{\mathcal{I}}$  with the positive orthant.  
 The model is parametrized by

$$V = M \cap \{x \in \mathbb{R}^{\mathcal{I}} : \Pi_{\mathcal{N}} x = c\}.$$



Interpretable parametrization: (conditional) expected cell counts.

# Maximum Likelihood Estimation

In log-linear models inference relies on MLE:

$$\hat{\theta} = \operatorname{argsup}_{\theta \in \mathbb{R}^{d-m}} p_{\theta}(n)$$

The MLEs  $\hat{\mu} \in \mathcal{M} \ominus \mathcal{N}$  and  $\hat{m} \in V$  are similarly defined.

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- If the supremum is not achieved the MLE does not exist. Instead supremum is realized in the limit
  - $\{\theta_n\} \subset \mathbb{R}^{d-m}: \|\theta_n\| \rightarrow \infty$
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- Far from being a just numerical issue. Existent MLE needed to
  - get correct asymptotic approximations to various goodness-of-fit testing statistics in regular and double-asymptotic setting;
  - obtain standard errors for the model parameters;
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  - carry out conditional inference.
- Nonexistence of the MLE leads to issues of estimability and assessment of the model complexity.

# Maximum Likelihood Estimation

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- Haberman's **pathological** example (1974).

	[12]	[13]	[23]
0			
			0

- In  $2^K$  table with positive entries set 2 cells to zero at random. Under the model of no-3-way interactions, a zero margin will occur with probability

$$\frac{k}{2^k - 1} \approx 0, \text{ for large } K,$$

and a nonexistent MLE leaving all margins positive with probability

$$\frac{2^{k-1} - k}{2^k - 1} \approx \frac{1}{2}, \text{ for large } K.$$

## Maximum Likelihood Estimation: Goals

- 1 Characterize patterns of sampling zeros leading to the nonexistence of the MLE.
- 2 Statistical consequence of a nonexistent MLE.
- 3 Algorithms.

## Basics of Discrete Exponential Families

See Barndorff-Nielsen (1974), Brown (1986), Jensen (1989),  
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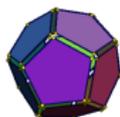
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- The set  $P = \text{convhull}(\mathcal{T})$  is called the **convex support** of  $\mathcal{E}$ .

- It is a polyhedron.



- $\text{int}(P) = \{\mathbb{E}_\theta[T], \theta \in \Theta\}$ : **mean value space**.
- $\text{int}(P)$  and  $\Theta$  are homeomorphic: **mean value parametrization**.

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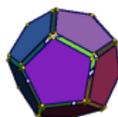
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## Existence of the MLE

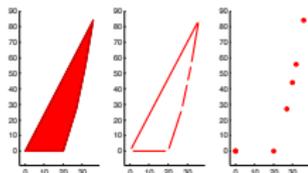
The MLE exists if and only if  $t \in \text{int}(P)$ .

## Extended Exponential Families: Geometric Construction

- For every face  $F$  of  $P$ , construct the exponential family of distributions  $\mathcal{E}_F$  for the sample points in  $F$  with convex support  $F$ . Note that  $\mathcal{E}_F$  depends on  $\dim(F) < d$  parameters only.

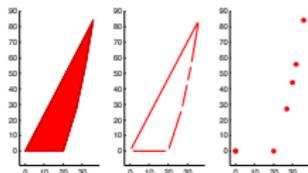
## Extended Exponential Families: Geometric Construction

- For every face  $F$  of  $P$ , construct the exponential family of distributions  $\mathcal{E}_F$  for the sample points in  $F$  with convex support  $F$ . Note that  $\mathcal{E}_F$  depends on  $\dim(F) < d$  parameters only.
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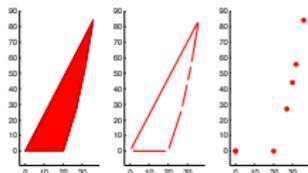
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### Extended Exponential Family

The extended exponential family is the closure of the original family. Geometrically, this corresponds to taking the closure of the mean value space, i.e. including the boundary of  $P$ .

## Convex Supports (Mean Value Parametrization)

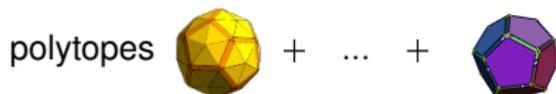
- Poisson sampling scheme: **marginal cone**  $C_A = \text{cone}(A)$  (Eriksson et al., 2006)



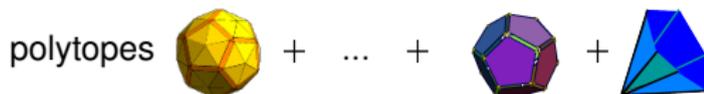
- Multinomial sampling scheme: **marginal polytope**  $\text{convhull}(A)$



- Product multinomial sampling scheme: Minkowski sum of convex



- Poisson-multinomial: Minkowski sum of polyhedral cone and convex



## Convex Supports (Mean Value Parametrization)

- $\text{int}(P)$  homeomorphic to  $V$ , with homeomorphism given by

$$x \in V \mapsto A^T x \in P,$$

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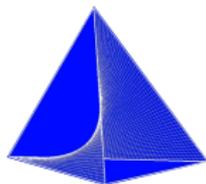
- $\text{int}(P)$  homeomorphic to  $V$ , with homeomorphism given by

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known as the **moment map**.

- Homeomorphism extended to the boundaries.

$\text{cl}(V)$  is also a mean value parametrization of  $\bar{\mathcal{E}}$ .



## Maximum Likelihood Estimation: Existence

### Existence of the MLE (assume minimality)

The MLE of  $\theta$  (or of  $\mu$  or of  $m$ ) exists (and is unique) if and only if  $A^T n \in \text{ri}(C_A)$  and satisfy the moment equations

$$\nabla\psi(\hat{\theta}) = A^T n$$

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- Application of standard theory of exponential families. Haberman (1974) first to derive it.
- Results apply to more general conditional Poisson sampling under additional condition.

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The following are equivalent
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## Existence of the MLE

The MLE does not exist if and only if  $\{i: n(i) = 0\} \supset \mathcal{F}^c$ , for a facial set  $\mathcal{F}$ .

## Examples: Likelihood Zeros – `polymake`

$2^2$  table and the model  $[12][13][23]$ .  
 $C_A$  has 16 facets, 12 of which correspond to null margins.

0	
0	


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0	0	
0	0	

0	0	
0	0	

		0

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0		
0	0	

	0	0
	0	

0		0
		0

## Examples: Likelihood Zeros – `polymake`

$4 \times 3 \times 6$  table and the model  $[12][13][23]$ .  
 $C_A$  has 153,858 facets, 54 of which correspond to null margins.

0		
0		0
0		0

	0	0
		0
0		0

	0	
	0	0
	0	0

	0	
	0	0
	0	0

	0	0
		0
0		0

0	0	
	0	
0		

## Examples: Likelihood Zeros – `polymake`

$2^4$  table and the non-graphical model  $[12][13][14][23][34]$ .  
 $C_A$  has 56 facets, 24 of which correspond to zero margins.

0	0
0	

0	

0	

	0

## Examples: Likelihood Zeros – `polymake`

$3^4$  table and the 4-cycle model [12][14][23][34].  
 $C_A$  has 1,116 facets, 16 of which correspond to zero margins.

0		0
		0

0	0	0
0	0	0
0	0	

0	0	0
	0	0
	0	

0		0
0	0	0
0	0	0

0		
0	0	0
0	0	

	0	0
	0	

0		0
		0
0	0	0

0		
0	0	

0	0	0
	0	0
0	0	0

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- The combinatorial complexity of  $P_v$  is large.  
**Example** the  $f$ -vector of  $P_8$  is (Stanley, 1991)

(334982, 1726648, 3529344, 3679872, 2074660, 610288, 81144, 3322).

The number of facets and of vertices of  $P_4$ ,  $P_5$ ,  $P_6$  and  $P_7$  are 22, 60, 224 and 882 and 46, 332, 2874 and 29874, respectively.

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- For the  $\beta$ -model, the convex support is the **polytope of degree sequences**:  $P_\nu \subset \mathbb{R}^\nu$ .

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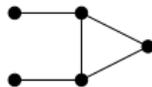
- **Cayley Trick**: Represent  $\beta$ -model as a log-linear model under product-multinomial constraints. Use a higher-dimensional marginal cone in  $\mathbb{R}^{\binom{\nu}{2} + \nu}$  with smaller complexity.

## Example: The $\beta$ -Model

- When  $v = 4$ , there are 14 facial sets corresponding to the facets of  $P_4$ , 8 of which associated to a degree of 0 or 3.



- For  $v = 5$ , example of a facial set for which the degrees are bounded away from 0 and 4.



- For  $v = 6$ , example of a facial set for which the degrees are bounded away from 0 and 5.



## Parameter Estimability

Assume the Poisson scheme and suppose that the MLE does not exist.

- $A^T n \in \text{ri}(F)$ , for some **random** face  $F$  of  $C_A$  of **random** dimension  $d_F$ .
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What can we do (estimate)?

- Let  $\mathcal{L}_F$  to be the subspace generated by the normal cone to  $F$ .  
Equivalence relation on  $\mathbb{R}^d$ :  $\theta_1 \sim^{\mathcal{L}_F} \theta_2$  if and only if  $\theta_1 - \theta_2 \in \mathcal{L}_F$ .  
Set  $\theta_{\mathcal{L}_F}$  for the equivalence class containing  $\theta$  and  $\Theta_{\mathcal{L}_F} = \{\theta_{\mathcal{L}_F}, \theta \in \mathbb{R}^d\}$ .
- Let  $\mathcal{F}$  the facial set associated to  $F$  and let  $\pi_{\mathcal{F}} : \mathbb{R}^{\mathcal{I}} \rightarrow \mathbb{R}^{\mathcal{F}}$  be the coordinate projection:

$$x \mapsto \{x(i) : i \in \mathcal{F}\}.$$

# Parameter Estimability

## Parameter Estimability

- (i) The family  $\mathcal{E}_F$  is non-identifiable: any two points  $\theta_1 \stackrel{\mathcal{L}_F}{\sim} \theta_2$  specify the same distribution.
- (ii) The family  $\mathcal{E}_F$  is parametrized by  $\Theta_{\mathcal{L}_F}$ , or, equivalently, by  $\pi_{\mathcal{F}}(\mathcal{M})$  and is of order  $d_F$ .
- (iii) The set  $\Theta_{\mathcal{L}_F}$  is a  $d_F$ -dimensional dimensional vector space comprised of parallel affine subspaces of  $\mathbb{R}^d$  of dimension  $\dim(\mathcal{L}_F) = d - d_F$ . It is isomorphic to  $\pi_{\mathcal{F}}(\mathcal{M})$ .

For product multinomial sampling schemes, replace

- $\mathcal{L}_F$  with  $\mathcal{L}_F + \{\zeta : A\zeta \in \mathcal{N}\}$ ;
- $\pi_{\mathcal{F}}(\mathcal{M})$  with  $\pi_{\mathcal{F}}(\mathcal{M} \ominus \mathcal{N})$ .

## Parameter Estimability

- For the extended family  $\mathcal{E}_F$  with corresponding facial set  $\mathcal{F}$ 
  - $\mathcal{M} \cap (\mathcal{N} + \mathcal{L}_F)^c$  is estimable
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- **Extended MLEs:**

- **Natural parametrization:** Reparametrize  $\mathcal{E}_F$  using a new design matrix  $A_{\mathcal{F}}$  with  $\mathcal{R}(A_{\mathcal{F}}) = \mathcal{M} \cap (\mathcal{N} + \mathcal{L}_F)^c$ . The extended MLE of the natural parameter is the MLE (which exists and is unique) of the corresponding family.
- **Mean value parametrization:** The extended MLE is the unique point

$$\hat{m} = \text{bd}(V) \cap \{x \geq 0 : A^{\top} x = A^{\top} n\},$$

where  $\text{supp}(\hat{m}) = \mathcal{F}$ .

- Correct model complexity: the **adjusted number of degrees of freedom** is

$$|\mathcal{F}| - d_F.$$

## Parameter Estimability: Examples

$2^3$  table and the model  $[12][13][23]$

0	

	0

$d_F = |\mathcal{F}| = 6$ : saturated model for  $\mathcal{E}_F$ !

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0		
0	0	

	0	0
	0	

0		0
		0

$d_F = |\mathcal{F}| = 18$ : saturated model for  $\mathcal{E}_F$ !

## Parameter Estimability: Examples

$3^3$  table and the model  $[12][13][23]$ . The red zeros are not likelihood zeros.

0		
0		

		0
	0	0

0		0
0		

$d_F = 18$ ,  $|\mathcal{F}| = 21$ : the number of adjusted degrees of freedom is 3.

## Parameter Estimability: Examples

$3^3$  table and the model [12][13][23]

	0	0
0		0
0	0	

0	0	
	0	0
0		0

0		0
0	0	
	0	0

The MLE exists!

## Parameter Estimability: Mildew Fungus Example

			1		2				D		
			1		2		1		2		E
			1	2	1	2	1	2	1	2	F
1	1	1	0	0	0	0	3	0	1	0	
		2	0	1	0	0	0	1	0	0	
	2	1	1	0	1	0	7	1	4	0	
		2	0	0	0	2	1	3	0	11	
2	1	1	16	1	4	0	1	0	0	0	
		2	1	4	1	4	0	0	0	1	
	2	1	0	0	0	0	0	0	0	0	
		2	0	0	0	0	0	0	0	0	
A	B	C									

## Parameter Estimability: Mildew Fungus Example

MIM (Edwards, 2000) selected optimal model using a greedy stepwise backward model selection procedure based on testing individual edges.



The final model is biologically plausible.

## Parameter Estimability: Mildew Fungus Example

Sequence of models found by MIM. Red boxes indicate zero margins (MLE does not exist).

Model	Unadjusted d.f.	Adjusted d.f.
[ABCDEF]	0	0
[ABCEF] [ABCDE]	16	3
[BCEF] [ABCDE]	24	6
[BCEF] [ABCE] [ABCD]	32	12
[BCEF] [ABCE] [ABD]	36	17
[BCEF] [AD] [ABCE]	38	18
[CEF] [AD] [ABCE]	42	22
[CEF] [AD] [BCE] [ABE]	46	27
[CEF] [AD] [ABE]	48	29
[CEF] [AD] [BE] [AB]	50	31
[CF][CE][AD] [BE] [AB]	52	37

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Two-step procedure:

- **Step 1**

Identify the facial set  $\mathcal{F}$  and compute a basis for  $\pi_{\mathcal{F}}(\mathcal{M} \cap (\mathcal{N} + \mathcal{L}_F)^c)$ .

To compute  $\mathcal{F}$ :

*Given  $\mathbf{t} = A^T n$ , determine the facial set  $\mathcal{F}$  of rows of  $A$  which span the face  $F$  of  $C_A$  such that  $\mathbf{t} \in \text{ri}(F)$ .*

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- **Step 2**

Optimize the restricted likelihood function for the extended family.  
When  $\mathcal{F}$  is available, this is equivalent to maximizing the likelihood of a log-linear model **with structural zeros along  $\mathcal{F}$** . (Easy)

## Algorithms for Extended Maximum Likelihood Estimation

Step 1 (finding  $\mathcal{F}$ ) is the important one.

- Let  $A_+$  and  $A_0$  the sub-matrix of  $A$  corresponding to positive and zero entries of  $n$ .

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- 
- This can be done with repeated iterations of LP (see also Geyer, 2009) or with non-linear methods.  
For large problems, they can be **computationally intensive**.

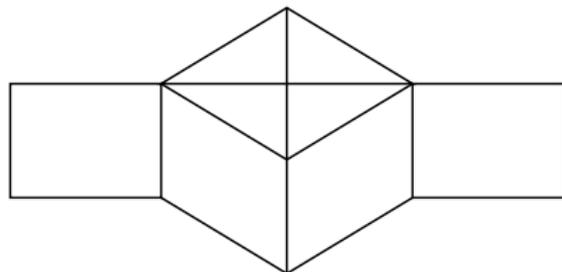
Relevance to exact inference: knowledge of  $\mathcal{F}$  can help finding Markov bases.

## Reducible Hierarchical Log-Linear Models

- For **reducible** hierarchical log-linear models both tasks can be carried out in parallel over appropriate sub-models.
- A hierarchical log-linear model (simplicial complex) is **reducible** if it can be obtained as the direct join of two sub simplicial complex (see Lauritzen, 1996). Apply the definition recursively.

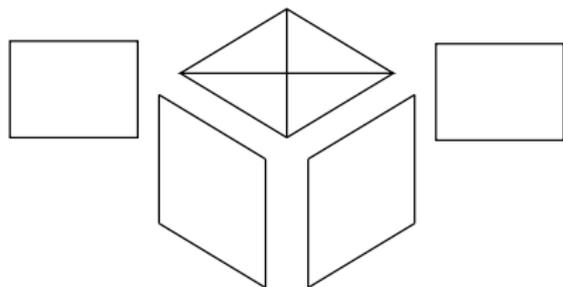
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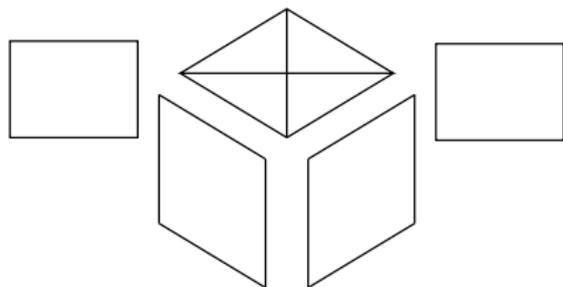
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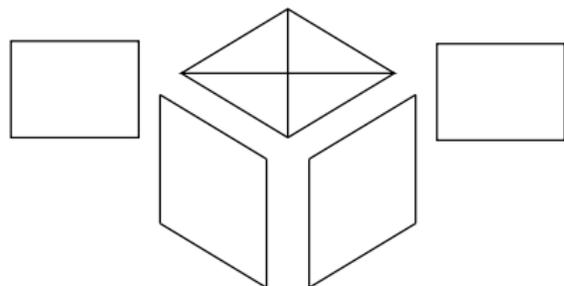
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- A hierarchical log-linear model (simplicial complex) is **reducible** if it can be obtained as the direct join of two sub simplicial complex (see Lauritzen, 1996). Apply the definition recursively.



- Theoretical justification: reducible models are defined by **cuts** (Barndorff-Nielsen, 1974).
- Old idea: Hara et al. (2011), Engström et al. (2011), Sullivant (2007), Eriksson et al. (2006), Dobra and Sullivant (2004), Badsberg and Malvestuto (2001), Frydenberg (1990), Leimer (1993), Tarjan (1985).

## Still lots of work ahead...

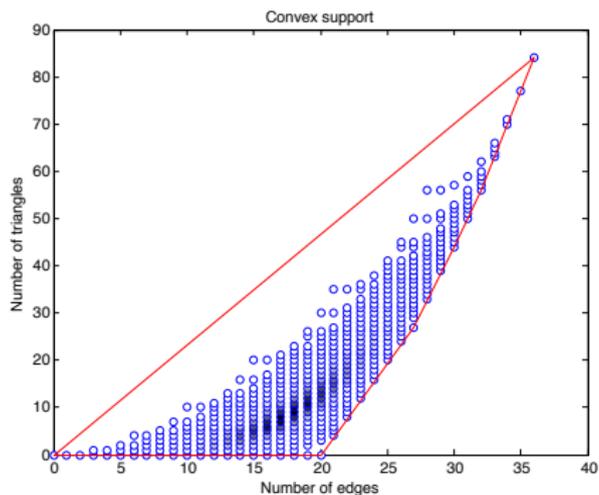
- The validity/applicability of model selection based on adjusted degree of freedom has to be investigated, especially in the **double asymptotic** framework.
  
- Computationally efficient methods for **model selection** for large tables still lacking.

## Still lots of work ahead...

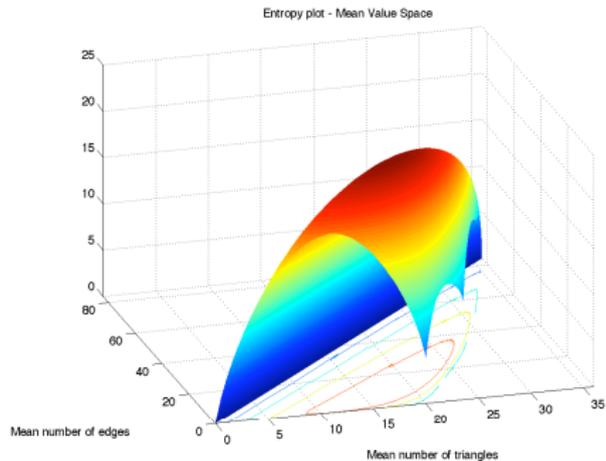
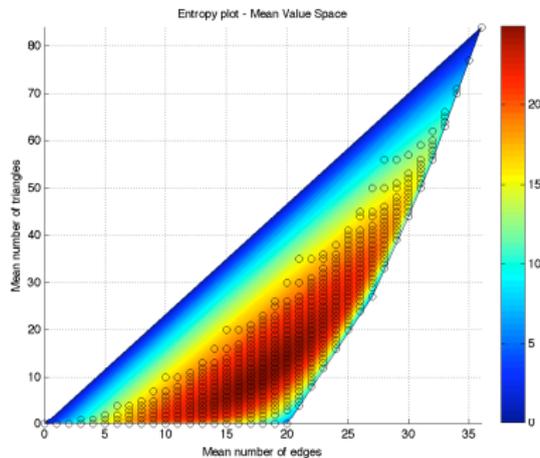
Thank you

- Fienberg S. E. and Rinaldo, A. (2011). Maximum Likelihood Estimation in Log-linear Models, <http://arxiv.org/abs/1104.3618>
- Rinaldo, A., Petrović, S. and Fienberg, S. E. (2011). Maximum Likelihood Estimation in Network Models, <http://arxiv.org/abs/1105.6145>
- Rinaldo, A., Fienberg, S. E. and Zhou, Y. (2009). On the Geometry of Discrete Exponential Families with Application to Exponential Random Graph Models, *Electronic Journal of Statistics*, 3, 446–484.

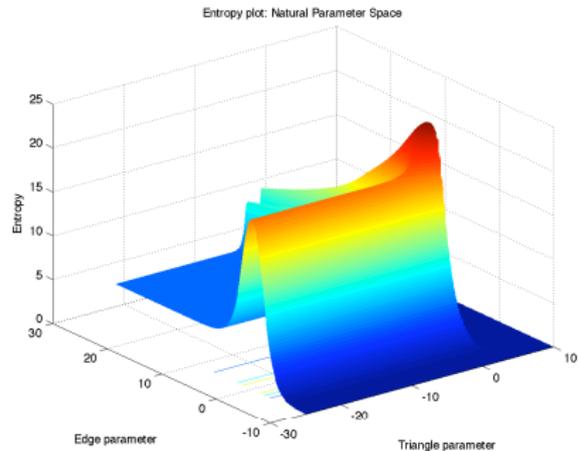
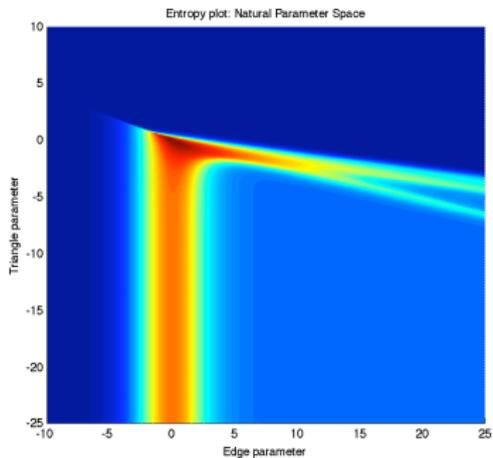
9 nodes: sufficient statistics are the number of edges and triangles.



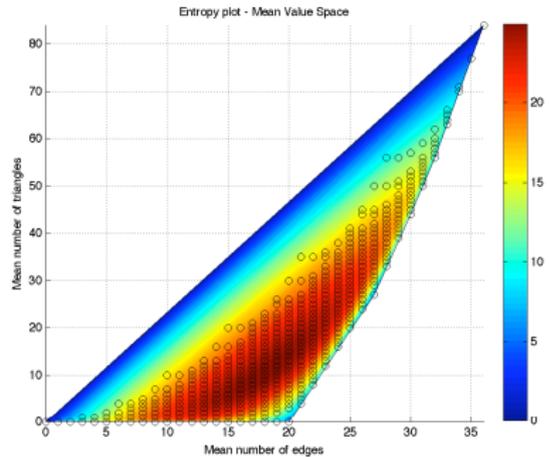
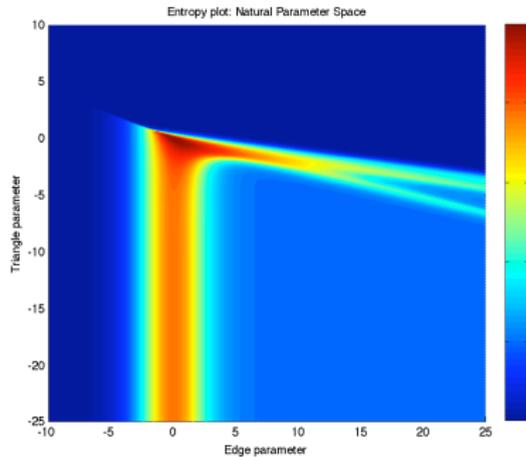
## Entropy plot over the mean value space.



Entropy plot over the natural parameter space.



## Entropy plots of the natural space and mean value spaces.



## Entropy plots of the natural space space with superimposed the normal fan and of the mean value space.

