Parametrizing graphical models

Graphical models: part 3 + algebra
Algebraic & Geometric Methods in Statistics

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Created for Math/Stat 561

Mar 31, 2026.

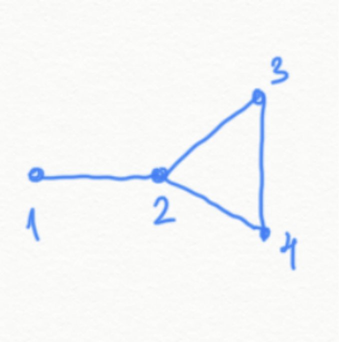
Factorization property

- We want to characterize **all** the distributions that satisfy the Markov properties for a *given graph*.
  - Hammersley-Clifford theorem relates the implicit description of a graphical model through Markov properties to a parametric description.
- Recall: definition of factorizing according to a graph via cliques. [board]
- Review Theorem 13.2.10 (recursive factorization in DAGs) with *proof*.

Question (example)

What are the maximal cliques of G?

1. $\{1\}$
2. $\{1, 2\}$
3. $\{1, 2, 3, \}$
4. $\{2, 3, 4\}$

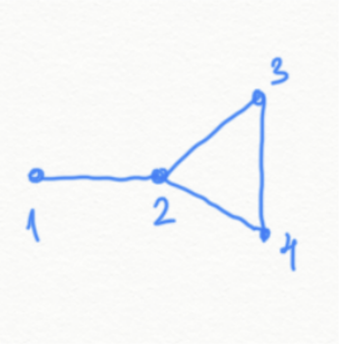


Question (example)

What are the maximal cliques of G?

1. $\{1\}$
2. $\{1, 2\}$
3. $\{1, 2, 3, \}$
4. $\{2, 3, 4\}$

Correct answers: 2 and 4.



Examples from 13.4

- (Homogeneous) Markov chain - example 13.4.1 and connection to chapter 1
- Hidden Markov model

[board notes] <- literally write out these 2 examples from the book! (Sonja: see file Lecture19-insert-book-AlgStas-Example13.4.1forLecture19.pdf in Dropbox)

Discrete distributions - and algebra&geometry

- $X = \{X_1, \ldots, X_m\}$ discrete random vector
- The distribution p on X factors according to G if

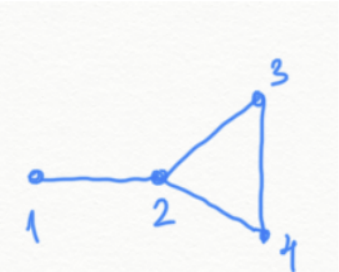
$$p_{i_1 i_2 \ldots i_m} \propto \prod_{C \in \mathcal{C}(G)} \theta^{(C)}_{i_C}.$$

- This is **a monomial parametrization**. Hence the set of distributions that factorize according to a graph G form a hierarchical **log-linear model**.

$C_{pairs} = \{1 \perp\!\!\!\perp 3|(2,4), 1 \perp\!\!\!\perp 4|(2,3)\}$.
$C_{global} = C_{pairs} \cup \{1 \perp\!\!\!\perp (3,4)|2\}$.

- Spell this out: [board]

$$p(x) = \frac{1}{Z}\theta^{(12)}_{i_1 i_2}\theta^{(234)}_{i_2 i_3 i_4}.$$



From Miles' notes:

- Theorem 3.1. (Hammersley-Clifford, factorization according to G)
- Proposition 3.1 (explicit clique factorization and log-linear models from graphs!)
- Example 3.4 (undirected- example of clique factorization)
- Example 3.4 (directed!)
- Theorem 3.2 (directed factorization)

Now we will cover the rest of these slides, as much as time allows, and finish them off after student presentations whenever time permits.

Agenda

1. Code for generating the minors and the statements from a graph (directed or undirected)
2. Binomials? Markov bases? **Connection**
3. Computing the MLE of an example graph $\mapsto$ homework 5

Figure 3.2.3: Directed graphs representing (a) $X_1 \perp\!\!\!\perp X_3 \mid X_2$ and (b) $X_1 \perp\!\!\!\perp X_2$.

Figure 1: Source: Oberwolfach lectures

- Here is an incredible online resource: Maathuis, Drton, Lauritzen & Wainwright's Handbook of graphical models

Part One

Code for generating the minors and the statements from a graph (directed or undirected)

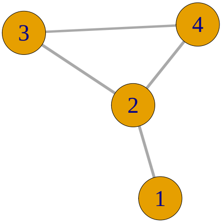
Global & Pairwise Markov proprety - algebra

$C_{pairs} = \{1 \perp\!\!\!\perp 3 | (2,4), 1 \perp\!\!\!\perp 4 | (2,3)\}$.
$C_{global} = C_{pairs} \cup \{1 \perp\!\!\!\perp (3,4) | 2\}$.

Question (example)

How many polynomials generate the corresponding CI ideal?

```
Warning: `graph()` was deprecat
i Please use `make_graph()` ins
This warning is displayed once
Call `lifecycle::last_lifecycle
generated.
```



- $M_1 = \begin{bmatrix} p_{0000} & p_{0001} & p_{0010} & p_{0011} \\ p_{1000} & p_{1001} & p_{1010} & p_{1011} \end{bmatrix}$
- $M_2 = \begin{bmatrix} p_{0100} & p_{0101} & p_{0110} & p_{0111} \\ p_{1100} & p_{1101} & p_{1110} & p_{1111} \end{bmatrix}$

Code for generating the polynomials (minors)

```
R1 = QQ[p_(0,0,0,0)..p_(1,1,1,1)]
M1 = matrix{{p_(0,0,0,0),p_(0,0,0,1),p_(0,0,1,0),p_(0,0,1,1)},
  {p_(1,0,0,0),p_(1,0,0,1),p_(1,0,1,0),p_(1,0,1,1)}}
M2 = matrix{{p_(0,1,0,0),p_(0,1,0,1),p_(0,1,1,0),p_(0,1,1,1)},
  {p_(1,1,0,0),p_(1,1,0,1),p_(1,1,1,0),p_(1,1,1,1)}}

--pairwise Markov property
IP = ideal(det(M1_{0,2}),det(M1_{1,3}),det(M2_{0,2}),
  det(M2_{1,3}),det(M1_{0,1}),det(M1_{2,3}),det(M2_{0,1}),det(M2_{2
--global Markov property
IG = minors(2,M1) + minors(2,M2)
```

Task

Run this code. What is the output? Compare to next page.

- *Reminder:* Look at slides 10 and 11 of **lecture 4** – `M2` code for computing ideals (minors) of given CI statements.
- We can compute the ideal I_G of a graphical model as follows:

```
i97 : loadPackage "GraphicalModels"
o97 = GraphicalModels
i99 : G = graph({{1,2},{2,3},{3,4},{2,4}})
o99 = Graph{1 => {2}       }
            2 => {1, 3, 4}
            3 => {2, 4}
            4 => {2, 3}
i100 : pairMarkov G
o100 = {{{1}, {4}, {2, 3}}, {{1}, {3}, {4, 2}}}
i101 : globalMarkov G
o101 = {{{1}, {3, 4}, {2}}}
-- This method displays only non-redundant statements.
```

. . . package shortcuts!!

```
i103 : R=markovRing(2,2,2,2);
i104 : conditionalIndependenceIdeal (R, pairMarkov(G)) / print;
- p        p         + p        p
   1,1,1,2 2,1,1,1      1,1,1,1 2,1,1,2
- p        p         + p        p
   1,1,2,2 2,1,2,1      1,1,2,1 2,1,2,2
- p        p         + p        p
   1,2,1,2 2,2,1,1      1,2,1,1 2,2,1,2
- p        p         + p        p
   1,2,2,2 2,2,2,1      1,2,2,1 2,2,2,2
- p        p         + p        p
   1,1,2,1 2,1,1,1      1,1,1,1 2,1,2,1
- p        p         + p        p
   1,1,2,2 2,1,1,2      1,1,1,2 2,1,2,2
- p        p         + p        p
   1,2,2,1 2,2,1,1      1,2,1,1 2,2,2,1
- p        p         + p        p
   1,2,2,2 2,2,1,2      1,2,1,2 2,2,2,2
```

Part Two

Binomials? Markov bases? **Connection**

The model of independence is a graphical model

Example 1.2.6 (Independence)**.** Let $\Gamma = [1][2]$. Then the hierarchical model consists of all positive probability matrices $(p_{i_1 i_2})$

$$p_{i_1 i_2} = \frac{1}{Z(\theta)} \theta^{(1)}_{i_1} \theta^{(2)}_{i_2}$$

where $\theta^{(j)} \in (0, \infty)^{r_j}$, $j = 1, 2$. That is, the model consists of all positive rank one matrices. It is the positive part of the model of independence $\mathcal{M}_{X \perp\!\!\!\perp Y}$, or in algebraic geometric language, the positive part of the Segre variety. $\square$

Figure 2: Oberwolfach Lectures

Example 3.1.10. Let X_1, X_2, X_3, X_4 be binary random variables, and consider the conditional independence model

$$\mathcal{C} = \{1 \perp\!\!\!\perp 3 \mid \{2,4\}, 2 \perp\!\!\!\perp 4 \mid \{1,3\}\}.$$

These are the conditional independence statements that hold for the graphical model associated to the four cycle graph with edges $\{12, 23, 34, 14\}$; see Section 3.2. The conditional independence ideal is generated by eight quadratic binomials:

$$\begin{aligned} I_{\mathcal{C}} &= I_{1 \perp\!\!\!\perp 3 \mid \{2,4\}} + I_{2 \perp\!\!\!\perp 4 \mid \{1,3\}} \\ &= \langle p_{1111}p_{2121} - p_{1121}p_{2111}, p_{1112}p_{2122} - p_{1122}p_{2112}, \\ &\quad p_{1211}p_{2221} - p_{1221}p_{2211}, p_{1212}p_{2222} - p_{1222}p_{2212}, \\ &\quad p_{1111}p_{1212} - p_{1112}p_{1211}, p_{1121}p_{1222} - p_{1122}p_{1221}, \\ &\quad p_{2111}p_{2212} - p_{2112}p_{2211}, p_{2121}p_{2222} - p_{2122}p_{2221} \rangle . \end{aligned}$$

The ideal $I_{\mathcal{C}}$ is radical and has nine minimal primes. One of these is a toric ideal I_Γ, namely the vanishing ideal of the hierarchical (and graphical) model associated to the simplicial complex $\Gamma = [12][23][34][14]$. The other eight components are linear ideals whose varieties all lie on the boundary of the probability simplex. In particular, all the irreducible components of the variety $V(I_{\mathcal{C}})$ are unirational. □

Figure 3: Oberwolfach Lectures

Hierarchical log-linear models

Definition [Simplicial complex]

Definition 9.3.1. For a set S, let 2^S denote its power set, that is, the set of all of its subsets. A *simplicial complex* with ground set S is a set $\Gamma \subseteq 2^S$ such that if $F \in \Gamma$ and $F' \subseteq F$, then $F' \in \Gamma$. The elements of Γ are called the *faces* of Γ and the inclusion maximal faces are the *facets* of Γ.

- We will use the bracket notation from the theory of hierarchical log-linear models
- $\Gamma = [12][13][23]$ is the bracket notation for the simplicial complex $\Gamma = \{\emptyset, \{1\}, \{2\}, \{3\}, \{1, 2\}, \{1, 3\}, \{2, 3\}\}$. The geometric realization of Γ is the boundary of a triangle.
- *Hierarchical models are log-linear models*, so they can be described as $\mathcal{M}_A$ for a suitable matrix A associated to the simplicial complex Γ. *Notation. . .*

Example 9.3.3 (Independence)**.** Let $\Gamma = [1][2]$. Then the hierarchical model consists of all positive probability matrices $(p_{i_1 i_2})$,

$$p_{i_1 i_2} = \frac{1}{Z(\theta)} \theta^{(1)}_{i_1} \theta^{(2)}_{i_2},$$

where $\theta^{(j)} \in (0, \infty)^{r_j}$, $j = 1, 2$. That is, the model consists of all positive rank one matrices. It is the positive part of the model of independence $\mathcal{M}_{X \perp\!\!\!\perp Y}$, or, in algebraic geometric language, the positive part of the Segre variety. The normalizing constant is

$$Z(\theta) = \sum_{i_1=1}^{r_1} \sum_{i_2=1}^{r_2} \theta_{i_1} \theta_{i_2}.$$

In this case, the normalizing constant factorizes as

$$Z(\theta) = \left(\sum_{i_1=1}^{r_1} \theta_{i_1} \right) \left(\sum_{i_2=1}^{r_2} \theta_{i_2} \right).$$

Complete factorization of the normalizing constant as in this example is a rare phenomenon.

Example 9.3.4 [no-3-factor interaction]

Γ=[12][13][23].
The hierarchical model $\mathcal{M}_\Gamma$ consists of all $r_1 \times r_2 \times r_3$ tables $(p_{i_1 i_2 i_3})$ with:

$$p_{i_1 i_2 i_3} = \frac{1}{Z(\theta)} \theta^{(12)}_{i_1 i_2} \theta^{(13)}_{i_1 i_3} \theta^{(23)}_{i_2 i_3},$$

for some positive real tables $\theta^{(12)} \in (0,\infty)^{r_1 \times r_2}$, $\theta^{(13)} \in (0,\infty)^{r_1 \times r_3}$, and $\theta^{(23)} \in (0,\infty)^{r_2 \times r_3}$.

- In the case of binary random variables, its implicit representation is given by the equation:

$$p_{111}p_{122}p_{212}p_{221} = p_{112}p_{121}p_{211}p_{222}.$$

The log-linear model consists of all positive probability distributions that satisfy this quartic equation.

Example - by hand.

Where are the "A" matrices??

Example 9.3.8 (Sufficient statistics of hierarchical models)**.** Returning to our examples above, for $\Gamma = [1][2]$ corresponding to the model of independence, the minimal sufficient statistics are the row and column sums of $u \in \mathbb{N}^{r_1 \times r_2}$. That is,

$$A_{[1][2]}u \;=\; (u|_1, u|_2).$$

- The recipe is the same as it was for other models on contingency tables! Columns are joint probabilities and rows are parameters:

Example 9.3.9 (Marginals of a 4-way table)**.** Let $\Gamma = [12][14][23]$ and $r_1 = r_2 = r_3 = r_4 = 2$. Then A_Γ is the matrix

	1111	1112	1121	1122	1211	1212	1221	1222	2111	2112	2121	2122	2211	2212	2221	2222
11··	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0
12··	0	0	0	0	1	1	1	1	0	0	0	0	0	0	0	0
21··	0	0	0	0	0	0	0	0	1	1	1	1	0	0	0	0
22··	0	0	0	0	0	0	0	0	0	0	0	0	1	1	1	1
1··1	1	0	1	0	1	0	1	0	0	0	0	0	0	0	0	0
1··2	0	1	0	1	0	1	0	1	0	0	0	0	0	0	0	0
2··1	0	0	0	0	0	0	0	0	1	0	1	0	1	0	1	0
2··2	0	0	0	0	0	0	0	0	0	1	0	1	0	1	0	1

,

These matrices are **huge**.

How are we ever going to compute anything, like a Markov basis for exact testing?!??

Citing Dobra 2003:

The statistical theory on graphical models (Madigan and York 1995; Whittaker 1990; Lauritzen 1996) shows that the conditional dependencies induced by a set of fixed marginals among the variables cross-classified in a table of counts can be visualized by means of an independence graph. In particular, a lot of attention has been given to **decomposable** graphs (Lauritzen 1996):

- a special class of graphs that can be '*broken*' into components such that
  1. every *component* is associated with *exactly one fixed marginal*, and
  2. *no information is lost* in the decomposition process, that is, no marginal is 'split' between two components.

Decomposable complexes

- Notation: $|\Gamma|$ = ground set of the complex Γ (the union of all faces).

Definition [decomposable complex] defn. 9.3.11.

A simplicial complex Γ is **reducible**, with reducible **decomposition** Γ_1, S, Γ_2 and **separator** $S \subset |\Gamma|$ if it satisfies $\Gamma = \Gamma_1 \cup \Gamma_2$ and $\Gamma_1 \cap \Gamma_2 = S$.
Furthermore, we assume here that neither Γ_1 nor Γ_2 is $= S$.
A simplicial complex is **decomposable** if it is reducible and Γ_1 and Γ_2 are decomposable or simplices.

Examples

- $[1][2] =$

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Examples

- [1][2] = decomposable
- [12][23][345] =

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Examples

- [1][2] = decomposable
- [12][23][345] = decomposable
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Examples

- [1][2] = decomposable
- [12][23][345] = decomposable
- [12][13][23] = not reducible.
- Γ = [12][13][23][345] is

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Furthermore, we assume here that neither Γ_1 nor Γ_2 is $= S$.
A simplicial complex is **decomposable** if it is reducible and Γ_1 and Γ_2 are decomposable or simplices.

Examples

- [1][2] = decomposable
- [12][23][345] = decomposable
- [12][13][23] = not reducible.
- Γ = [12][13][23][345] is reducible but not decomposable, with decomposition ([12][13][23], $\{3\}$, [345]).
- Any complex with only *two* facets is decomposable.

Markov bases of decomposable models

- If Γ is decomposable, then the Markov bases can be computed using a divide-and-conquer algorithm (via the decomposition).
  - The upshot is that they are all *quadratic* - degree $= 2$!
  - See Corollary 9.3.18, Example 9.3.19., but notation :(:(

Adrian Dobra 2003: *We show that primitive data swaps or moves are the only moves that have to be included in a Markov basis that links all the contingency tables having a set of fixed marginals when this set of marginals induces a decomposable independence graph. We give formulae that fully identify such Markov bases and show how to use these formulae to dynamically generate random moves.*

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- Good/bad news:
  - What do you think about the quartic from Example 9.3.4:

  Γ=[12][13][23] has the following implicit description:

  $p_{111}p_{122}p_{212}p_{221} = p_{112}p_{121}p_{211}p_{222}$.

Why is this degree > 2? . . . Is this model decomposable?

Question to ponder.

Why is [12][23][13] not a cycle?

How are complexes and graphs related?

The usual... license

This document is created for Math/Stat 561, Spring 2023.

Sources: textbook, *Kaie Kubjas*' Algebraic Statistics course at Aalto University.