SCORE EQUIVALENCE & POLYHEDRAL APPROACHES TO LEARNING BAYESIAN NETWORKS

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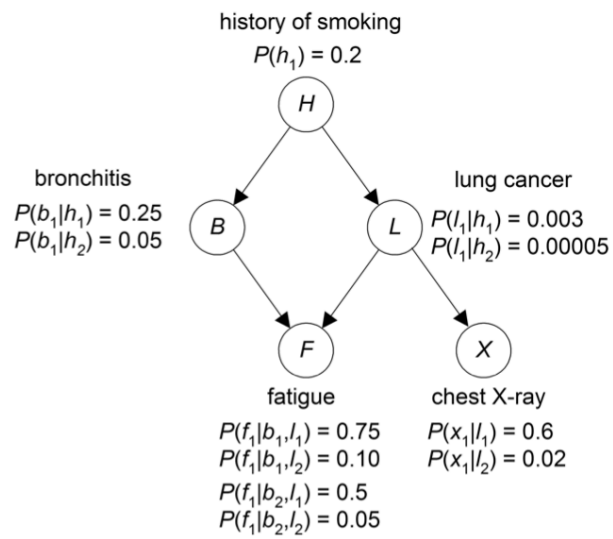
Definition

- A Bayesian network is a graphical model that represents a set of random variables and their conditional dependencies via a directed acyclic graph (DAG).



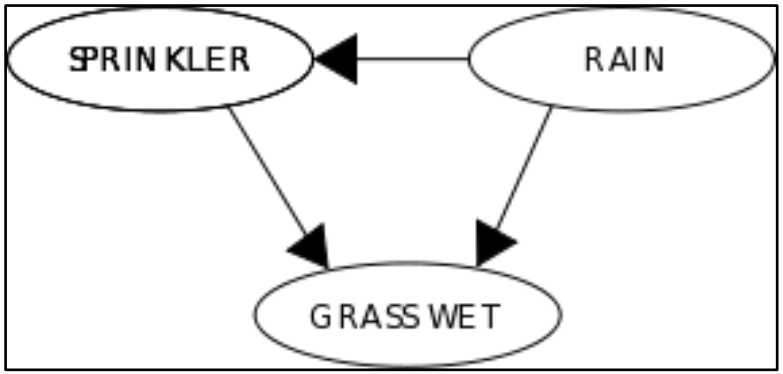
- Nodes → Random variables
  Edges → Conditional dependencies

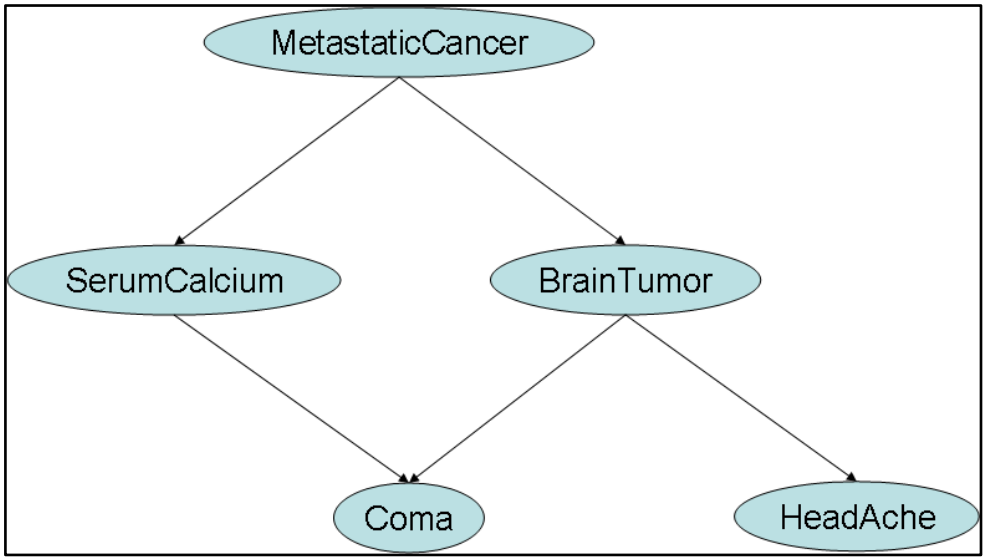
- Node (RV) is conditionally independent of its non-descendents; given the state of all its parents. *or*

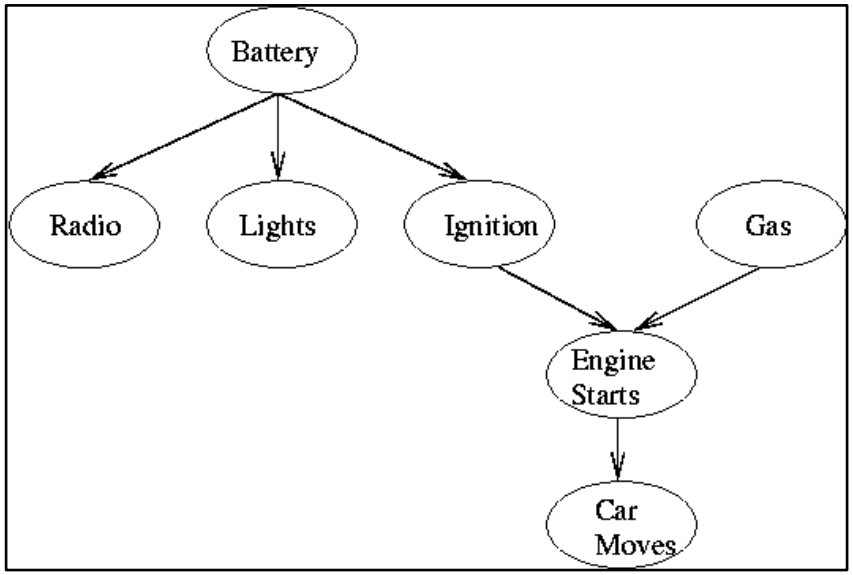
- Node (RV) is conditionally independent of all other nodes j, given its Markov blanket.

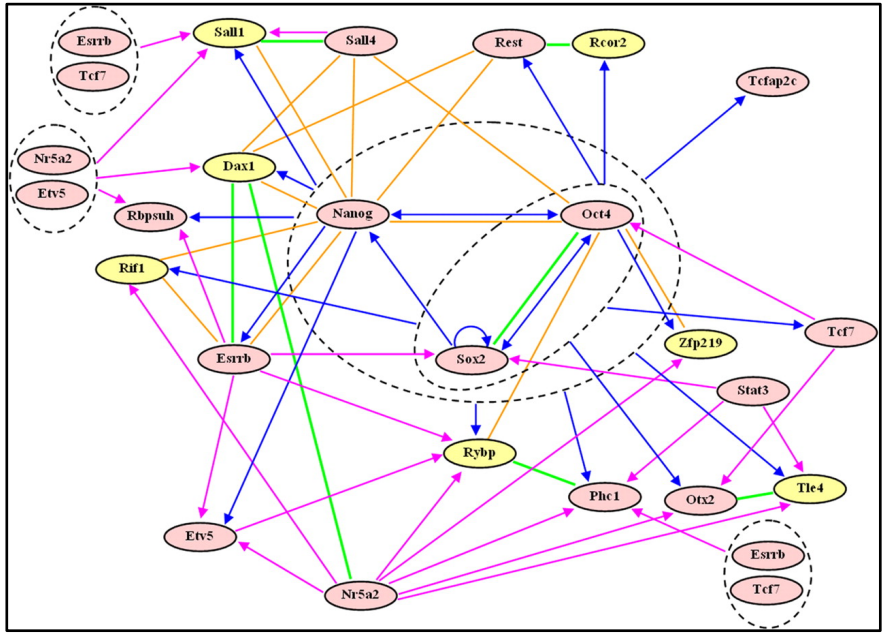
- Variables X, Y are conditionally independent (CI) given Z if Pr(X and Y | Z) = Pr(X | Z) Pr(Y | Z).

Examples


SPRINKLER
RAIN
GRASS WET


MetastaticCancer
SerumCalcium
BrainTumor
Coma
HeadAche


Battery
Radio
Lights
Ignition
Gas
Engine Starts
Car Moves


Esrrb
Tcf7
Sall1
Sall4
Rest
Rcor2
Tcfap2c
Nr5a2
Etv5
Dax1
Rbpsuh
Nanog
Oct4
Rif1
Tcf7
Esrrb
Sox2
Zfp219
Stat3
Rybp
Phc1
Otx2
Tle4
Etv5
Esrrb
Tcf7
Nr5a2

Learning Bayesian Network

Variables

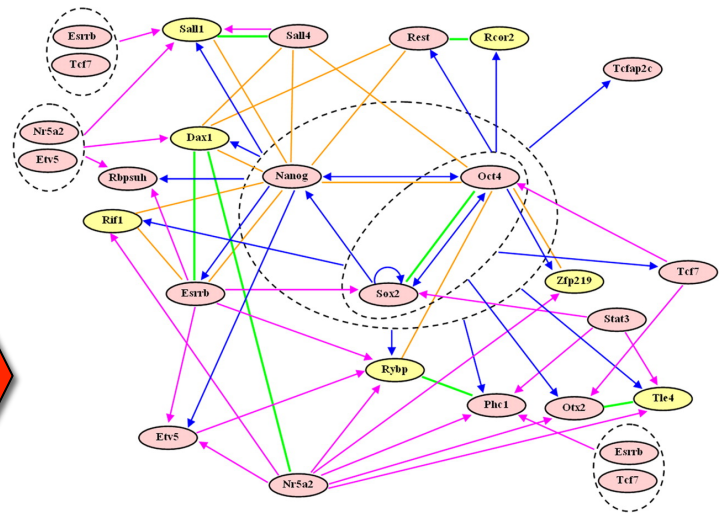
Observations

$$
\begin{bmatrix}
0 & 1 & 2 & 2 & 0 & 0 & 0 & 2 & 0 & \cdots \\
1 & 0 & 3 & 2 & 2 & 2 & 1 & 0 & 1 & \cdots \\
1 & 1 & 0 & 1 & 1 & 1 & 0 & 2 & 3 & \cdots \\
2 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 1 & \cdots \\
0 & 0 & 1 & 0 & 1 & 1 & 2 & 1 & 0 & \cdots \\
2 & 1 & 2 & 1 & 0 & 1 & 0 & 2 & 2 & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots
\end{bmatrix}
$$

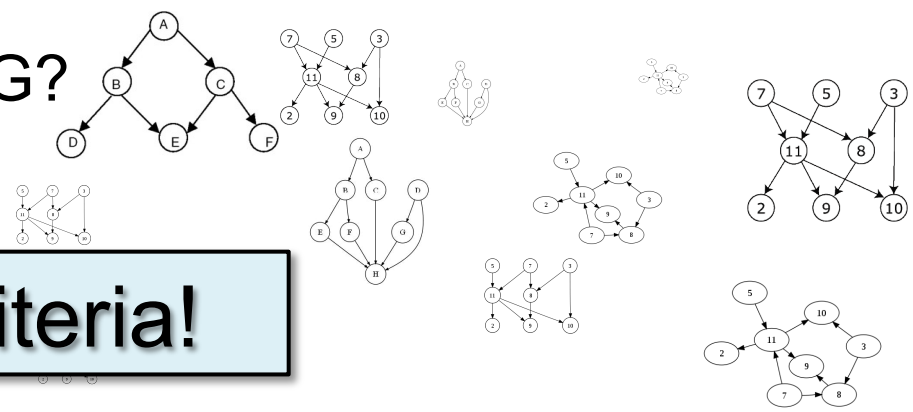
Learn

NP-Hard

"Best" Bayesian Network



How to find right DAG?



Scoring criteria!

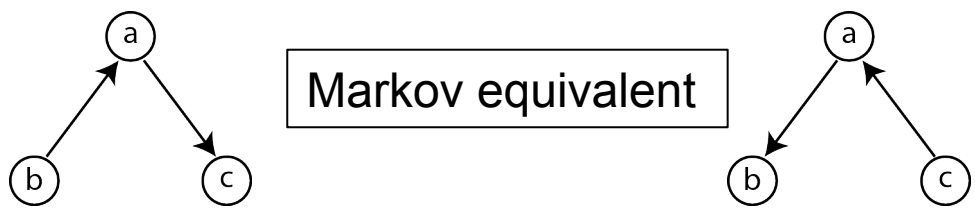
Scoring Criteria

- A scoring function Q(G, *D)* evaluates how well a DAG explains the data.
- We will only consider score equivalent and decomposable scoring functions
  - Bayesian Information Criterion (**BIC**),
  - Bayesian Dirichlet Equivalent (**BDE**).

Roughly: Likelihood of graph given data + penalty for complex graphs.

- Score equivalent: Score of two Markov equivalent graphs are the same.

WARNING: Two different DAGs may represent the same probability model! If so, they are called Markov equivalent.



Score Decomposable

A scoring function is score decomposable if there exists a set of functions (local scores)

$$q_{i|B} : DATA(\{i\} \cup B, d) \rightarrow \mathbb{R}$$

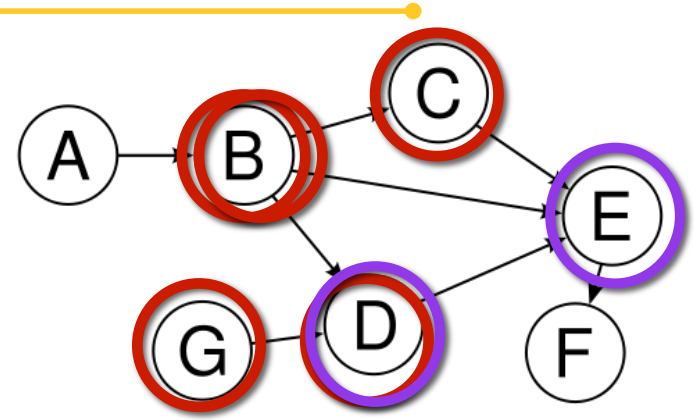
such that

Parents of node i in graph G.

$$\mathcal{Q}(G, D) = \sum_{i \in N} q_{i|pa_G(i)}(D_{\{i\} \cup pa_G(i)})$$

Sum over random variables / nodes.

Local score

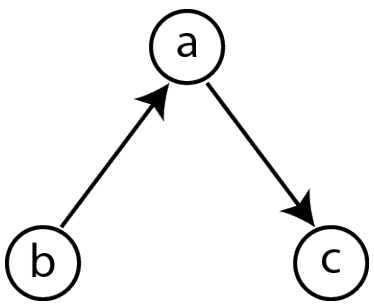


Score DAGs by summing the local score of each node and its parents!

Family Variable Representation

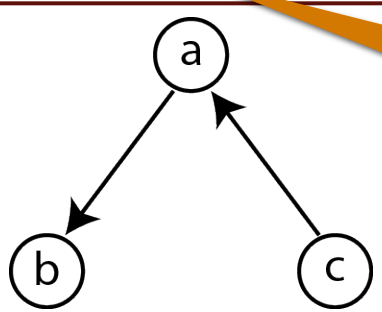
Given DAG G over variables N one has

$$\eta_G(i|B) = 1 \Leftrightarrow B = pa_G(i), \quad \eta_G(T) = 0 \text{ otherwise}$$



Record each nodes parent set!

$$\begin{array}{cc} & \begin{array}{cccccccccccc} a|\emptyset & a|b & a|c & a|bc & b|\emptyset & b|a & b|c & b|ac & c|\emptyset & c|a & c|b & c|ab \end{array} \\ \eta_G = & \begin{pmatrix} 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} \end{array}$$



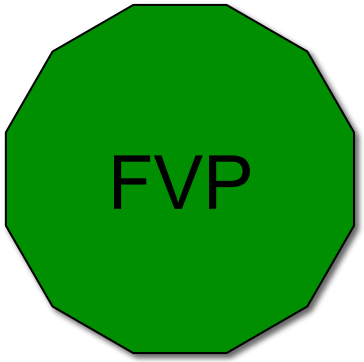
Two graphs are Markov equivalent, but different DAG representations!

$$\begin{array}{cc} & \begin{array}{cccccccccccc} a|\emptyset & a|b & a|c & a|bc & b|\emptyset & b|a & b|c & b|ac & c|\emptyset & c|a & c|b & c|ab \end{array} \\ \eta_G = & \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix} \end{array}$$

Family Variable Polytope (FVP)

$$\mathcal{P}_\eta := conv\{\eta_G \mid G \in \text{DAGs on } N\}$$

- Vertex ←→ DAG
- Dimension = $N(2^{(N-1)}-1)$
- Facet description for N=1,2,3,4
- No facet description N > 4
- Some facets known N > 4
- Simple IP relaxation
- IP solution gives DAG



Characteristic Imset Representation -Studeny

Goal: Unique vector representation of Markov equivalent classes of DAGs.

Notation: Suppose N random variables. We index the components of $v \in \mathbb{R}^{|N|}$ using subsets $T \subseteq N$, such as

$$v(T)$$

$N = \{a, b, c\}$

$$v = \begin{array}{c} \begin{array}{cccccccc} \emptyset & a & b & c & ab & ac & bc & abc \end{array} \\ \begin{pmatrix} 0, & 0, & 1, & 0, & 1, & 1, & 0, & 1 \end{pmatrix} \end{array}$$

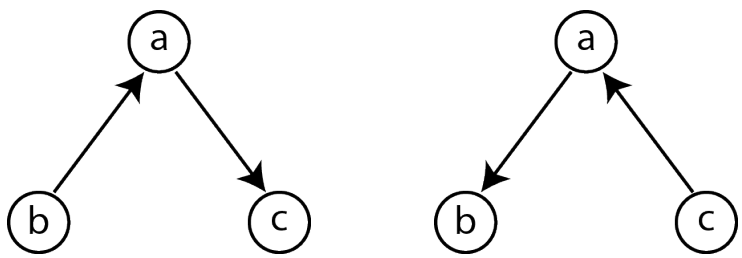
$$v(b) = 0,\ v(ac) = 1, \ldots$$

Characteristic Imset Representation

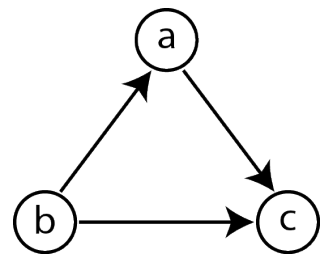
Given DAG G over variables N one has $c_G(T) \in \{0,1\}$ for any $T \subseteq N$, $|T| \geq 2$. Moreover

$$c_G(T) = 1 \text{ if and only if there exists } i \in T \text{ with } T \setminus \{i\} \subseteq pa_G(i).$$

Parents of node i in G.



$$c_G = \begin{array}{cccc} ab & ac & bc & abc \\ \end{array}$$
$$c_G = \begin{pmatrix} 1 & 1 & 0 & 0 \end{pmatrix}$$



$$c_G = \begin{array}{cccc} ab & ac & bc & abc \\ \end{array}$$
$$c_G = \begin{pmatrix} 1 & 1 & 1 & 1 \end{pmatrix}$$

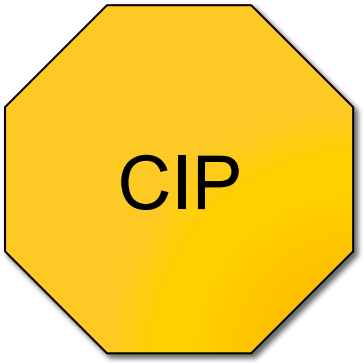
Theorem (Studeny, Hemmecke, Lindner 2011):

Characteristic imsets $\leftrightarrow$ Markov equivalence classes.

Characteristic Imset Polytope (CIP)

$$\mathcal{P}_c := conv\{c_G \mid G \in \text{DAGs on } N\}$$

- Vertex ←→ Markov Eq. Class
- Dimension = $2^N - N - 1$
- Facet description for N=1,2,3,4
- No facet description N > 4
- Some facets known N > 4
- Complex IP relaxation
- IP solution gives eq. class



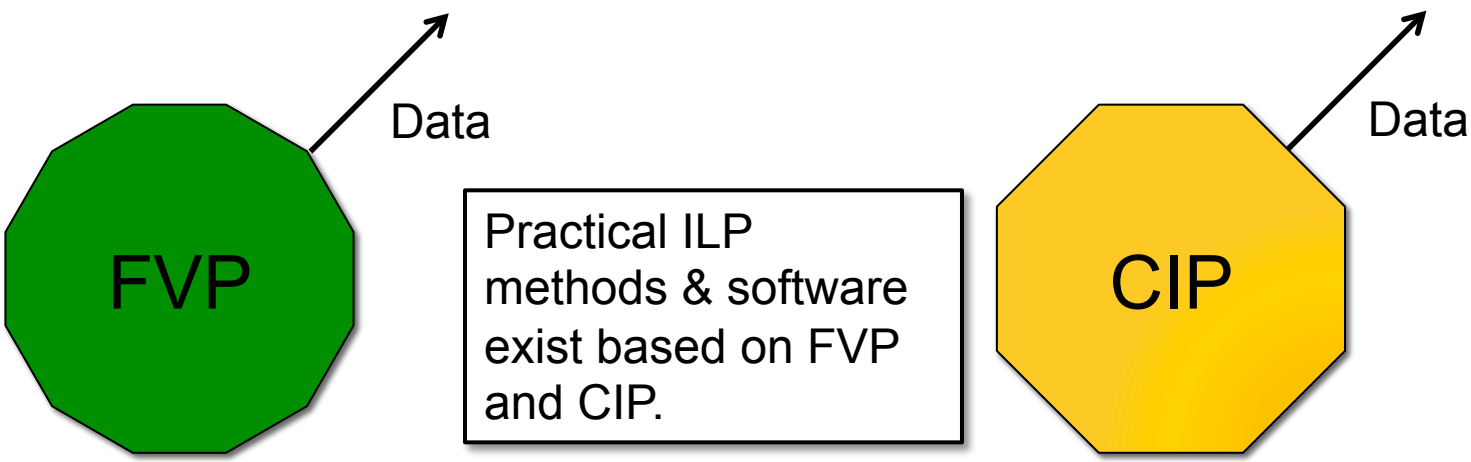
Geometric Approach to Learning BN

Every reasonable scoring function (BIC, BDE, …) is an affine function of family variable or char imset:

$$\mathcal{Q}(G, D) = \hat{s}_D^{\mathcal{Q}} - \langle \hat{t}_D^{\mathcal{Q}}, \eta_G \rangle = s_D^{\mathcal{Q}} - \langle t_D^{\mathcal{Q}}, c_G \rangle$$

Integer and linear programming techniques can be applied!

(Linear relaxations combined with row-generation and Brach-and-Cut)



FVP: Some Known Faces

- Order faces (Cussens et al.)

DAGs consistent with total order

- Sink faces (Cussens et al.)

DAGs with sink j

- Non-negative inequalities on family variables. (H., Cussens, Studeny).
- Modified convexity constraints (H, Cussens Studeny).

Node i has at most one parent set.

- Generalized cluster inequalities (H, Cussens, Studeny), (Cussens, et al.)

Coming up…

- Connected matroids on $C \subseteq N$, $|C| \geq 2$ (Studeny).
- Extreme supermodular set functions (H, Cussens, Studeny).

Coming up…

Super-modular Set Functions

DEFINITION 5.5 (standardized supermodular function). Any vector $m \in \mathbb{R}^{\mathcal{P}(N)}$ can be viewed as a real set function $m : \mathcal{P}(N) \to \mathbb{R}$. Such a set function is called *standardized* if $m(S) = 0$ for $S \subseteq N$, $|S| \leq 1$, and *supermodular* if

$$\forall U, V \subseteq N \quad m(U) + m(V) \leq m(U \cup V) + m(U \cap V)\,. \tag{5.4}$$

- The set of super-modular vectors is a polyhedral cone.
- Cone is pointed => it has finitely many extreme rays.
- Extreme rays correspond to faces of FVP.

- Remark: The rank functions of connected matroids are extreme rays of non-decreasing submodular functions (mirrors to supermodular functions).

Cluster Inequalities

$$\forall\, C \subseteq N,\ |C| > 1 : \qquad \sum_{a \in C} \sum_{B \cap C} \eta(a \,|\, B) \leq |C| - 1 \Big\}$$

- **Why?** Not all nodes in the cluster C can have a parent which is also in the cluster C

REMARK 3.2. The cluster inequalities do not allow cycles: consider a digraph G which has a cycle $i_1 \to \cdots \to i_p \to i_1$ and note that the cluster inequality with $C := \{i_1, \ldots, i_p\}$ would be violated.

Generalized Cluster Inequalities

- For every cluster $C \subseteq N$, $|C| > 2$ and $k = 1, \ldots, |C| - 1$ the **generalized cluster inequality** is

$$\sum_{a \in C} \sum_{\substack{B \subseteq N \setminus a: \\ |B \cap C| \geq k}} \eta(a \mid B) \leq |C| - k.$$

- **Why?** For any DAG G the induced subgraph G_C is acyclic and the first k nodes in C in a total order consistent with G_C has at most k-1 parents in C.

Connecting FVP and CIP

Linear map between Family variable and Char Imset: (Studeny, Haws)

$$\mathsf{c}_\eta(S) = \sum_{i \in S} \sum_{B,\, S\setminus\{i\} \subseteq B \subseteq N\setminus\{i\}} \eta(i \,|\, B) \qquad \text{for any } S \subseteq N,\ |S| \geq 2.$$

BIC & BDE always give SE obj!

$x \in FVP$ objective is score equivalent(SE) if

$$\forall\, G, H \in \mathsf{DAGS}\,(N) \quad G \sim H \;\Rightarrow\; \langle x, \eta_G \rangle = \langle x, \eta_H \rangle\,.$$

Face $F \in FVP$ is score equivalent if there exists a SE objective defining F.

A face $F \in FVP$ is weakly equivalent(WE) if

$$\forall\, G, H \in \mathsf{DAGS}\,(N) \quad G \sim H \qquad \eta_G \in F \quad \Rightarrow \quad \eta_H \in F\,.$$

Score Equivalence, FVP, & CIP

- **Theorem** [H, Cussens, Studeny]
  The following conditions are equivalent for a facet
  $$S \subseteq DAGS(N)$$
  a) S is closed under Markov equivalence
  b) S contains the whole equivalence class of full graphs
  c) S is SE
- **Corollary** [H, Cussens, Studeny]
  There is a 1-1 correspondence between SE faces of FVP and faces of CIP which preserves inclusion.
- **Corollary** [H, Cussens, Studeny]
  SE facets of the FVP correspond to those facets of the CIP that contain the 1-imset. None of those facets of CIP include the 0-imset. Moreover, these facets correspond to extreme supermodular functions.

Sufficiency of Score Equivalent Faces

- Learning BN structure = optimizing SE obj over FVP
- Are SE faces of FVP sufficient? Yes!
- **Theorem** [H, Cussens, Studeny]
  Let o be an SE objective. Then the LP problem of

$$\text{maximize } \eta \mapsto \langle o, \eta \rangle \text{ over } \eta \in FVP$$

  has the same optimal value as the LP problem to maximize the same function over the polyhedron
  - SE **faces** of FVP corresponding to facets of CIP not containing 0-imset
  - Non-negativity and modified convexity constraints.
- Not true for SE-**facets**! ☹ Must use all SE-faces.

Open Conjecture…something to think on

(H, Cussens, Studeny)

Theorem: Every weakly equivalent facet of family-variable polytope is a score equivalent facet.

(Haws, Cussens, Studeny)

Conjecture: Every weakly equivalent face of family-variable polytope is a score equivalent face.

Believe false, but counter-example must be in N >=4. Already performed extensive searches in N=4,5. ☹

THANK YOU!

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Polyhedral Approaches to Learning Bayesian Networks, David Haws, James Cussens, Milan Studeny, to appear in book on “Special Session on Algebraic and Geometric Methods in Applied Discrete Mathematics”, 2015.