On Geometric Approach to Structural Learning Bayesian Nets

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based on joint work with Jiří Vomlel and Raymond Hemmecke

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group "Decision Making and Control under Uncertainty"
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Summary of the talk

1. The idea of structural learning Bayesian nets
2. Algebraic approach
3. Geometric view
4. A short trip to convex geometry
5. Recent results and conjectures
6. Conclusions

Motivation: Bayesian networks

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In probabilistic expert systems, the structure (= the graph) was typically provided by an expert, but later, people became interested in the question of how to learn structure from statistical data.

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Traditional unique graphical representative of a BN structure is a special chain graph, called the *essential graph*. It (somehow) encodes shared features of acyclic directed graphs defining the structure.

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Definition

By a *quality criterion*, also named a *score metric* or a *score*, is meant a special real function $\mathcal{Q}$ of the BN structure, usually represented by a graph G, and of the database D. That is, $\mathcal{Q} : \mathrm{DAGS}\,(N) \times \mathrm{DATA}\,(N,d) \mapsto \mathbb{R}$.

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A quality criterion should be *statistically consistent*, but there are other reasonable requirements.

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There are two other important technical requirements on a quality criterion $\mathcal{Q}$ brought in connection with the maximization problem. One of them is that $\mathcal{Q}$ should be *score equivalent* (Bouckaert 1995), the other is that $\mathcal{Q}$ should be *decomposable* (Chickering 2002).

R.R. Bouckaert (1995). Bayesian belief networks: from construction to evidence. PhD thesis, University of Utrecht.

D.M. Chickering (2002). Optimal structure identification with greedy search. *Journal of Machine Learning Research* **3**: 507-554.

Algebraic approach: idea

The basic idea of an algebraic approach to learning BN structures (Studený 2005) is to represent both the BN structure and the database by a real vector.

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The crucial point is that the standard imset is a unique (algebraic) representative of the BN stucture and that every score equivalent and decomposable criterion $\mathcal{Q}$ is an affine function (= linear function plus a constant) of the standard imset.

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$$\langle m, u \rangle \equiv \sum_{A \subseteq N} m(A) \cdot u(A) \,.$$

Algebraic approach: standard imset

Given $A \subseteq N$, the symbol δ_A will denote a special imset given by:

$$\delta_A(B) = \begin{cases} 1 & \text{if } B = A, \\ 0 & \text{if } B \neq A, \end{cases} \qquad \text{for} \quad B \subseteq N.$$

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The *standard imset* for an acyclic directed graph G is given by the formula

$$u_G = \delta_N - \delta_\emptyset + \sum_{a \in N} \{\delta_{pa_G(a)} - \delta_{\{a\} \cup pa_G(a)}\}.$$

Here $pa_G(a) \equiv \{b \in N;\ b \to a \text{ in } G\}$ denotes the set of *parents* of the node a.

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Because every standard imset has at most $2 \cdot |N|$ non-zero values, it can be represented in the memory of a computer *with polynomial complexity* with respect to $|N|$.

Standard imsets: main observations

Standard imset is another uniquely determined representative of a BN structure. Actually, there exists a polynomial algorithm which translates the standard imset into the essential graph and conversely:

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Theorem (Studený 2005)

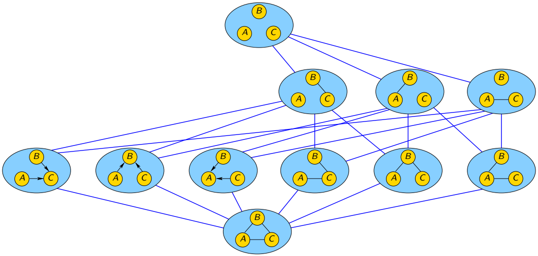
Let $\mathcal{Q}$ be a score equivalent and decomposable criterion, G any acyclic directed graph over N and D a database (over N). Then one has

$$\mathcal{Q}(G,D) = s_D^{\mathcal{Q}} - \langle t_D^{\mathcal{Q}}, u_G \rangle \,, \qquad \text{where } s_D^{\mathcal{Q}} \in \mathbb{R},$$

$t_D^{\mathcal{Q}}$ is a real vector in $\mathbb{R}^{\mathcal{P}(N)}$ and $\langle *, * \rangle$ denotes the scalar product. The vector $t_D^{\mathcal{Q}}$ is named the *data vector* (relative to $\mathcal{Q}$).

Example: the case of three variables

In the case of 3 variables one has 11 BN structures breaking into 5 types.



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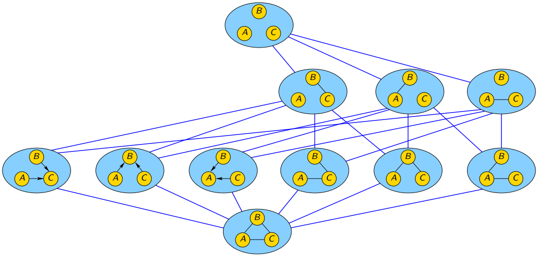

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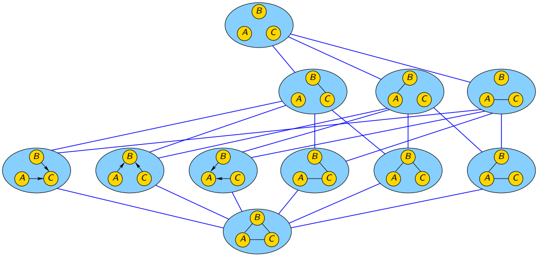

- The zero imset corresponds to the complete (undirected) essential graph.
- Six "elementary" imsets break into two types, namely $\delta_{ab} + \delta_{\emptyset} - \delta_a - \delta_b$ (encodes $a \perp\!\!\!\perp b | \emptyset$) and $\delta_{abc} + \delta_c - \delta_{ac} - \delta_{bc}$ (encodes $a \perp\!\!\!\perp b | c$); the respective essential graphs are $a \rightarrow c \leftarrow b$ and $a — c — b$.

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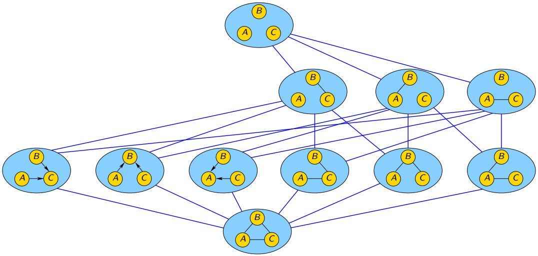

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- Three "semi-elementary" imsets of the form $\delta_{abc} + \delta_{\emptyset} - \delta_{a} - \delta_{bc}$ (encodes $a \perp\!\!\!\perp bc|\emptyset$) define one type; the respective graphs have just one edge.

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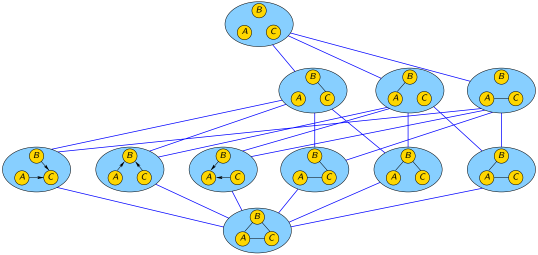

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- The imset $\delta_N - \sum_{i \in N} \delta_i + 2 \cdot \delta_{\emptyset}$ corresponds to the empty essential graph.

Geometric view

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This is a crucial observation made in a recent paper:

Theorem (Studený Vomlel Hemmecke 2010)

Having N fixed, none of the standard imsets is the convex combination of others. In particular, the set of standard imsets over N is the set of vertices (= extreme points) of a polytope $\mathsf{P} \subseteq \mathbb{R}^{\mathcal{P}(N)}$.

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$$\mathsf{H}^+ = \{\mathbf{x} \in \mathbb{R}^K ;\ \langle \mathbf{v}, \mathbf{x} \rangle \leq \alpha\},$$

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This is a fundamental result in convex geometry (not easy to prove).

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They are several computer packages that allow one to change between these two types of description of a polytope.

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A *face* F of a polytope $\mathsf{P} \subseteq \mathbb{R}^K$ is the intersection of P with a hyperplane isolating it:

$$\mathsf{F} = \mathsf{P} \cap \mathsf{H} \quad \text{where} \quad \text{either} \quad \mathsf{P} \subseteq \mathsf{H}^{+} \equiv \{\mathbf{x} \in \mathbb{R}^K;\ \langle \mathbf{v}, \mathbf{x} \rangle \leq \alpha\},$$
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$$\text{or} \quad \mathsf{P} \subseteq \mathsf{H}^- \equiv \{\mathbf{x} \in \mathbb{R}^K;\ \langle \mathbf{v}, \mathbf{x} \rangle \geq \alpha\}\,.$$

Of course, every face F of a polytope P is again a polytope.

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Definition (face)

By an *affine hyperplane* in $\mathbb{R}^K$ is meant any set of the form

$$\mathsf{H} = \{\mathbf{x} \in \mathbb{R}^K;\ \langle \mathbf{v}, \mathbf{x} \rangle = \alpha\} \qquad \text{where } 0 \neq \mathbf{v} \in \mathbb{R}^K \text{ and } \alpha \in \mathbb{R}\,.$$

A *face* F of a polytope $\mathsf{P} \subseteq \mathbb{R}^K$ is the intersection of P with a hyperplane isolating it:

$$\mathsf{F} = \mathsf{P} \cap \mathsf{H} \quad \text{where} \quad \text{either} \quad \mathsf{P} \subseteq \mathsf{H}^+ \equiv \{\mathbf{x} \in \mathbb{R}^K;\ \langle \mathbf{v}, \mathbf{x} \rangle \leq \alpha\},$$
$$\text{or} \quad \mathsf{P} \subseteq \mathsf{H}^- \equiv \{\mathbf{x} \in \mathbb{R}^K;\ \langle \mathbf{v}, \mathbf{x} \rangle \geq \alpha\}\,.$$

Of course, every face F of a polytope P is again a polytope.

Faces can be classified by their dimensions. The most important are *vertices* (= extreme points), *edges* and *facets*.

The outer description of a polytope corresponds to its facets.

Linear programming and simplex method

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Again, there are efficient software packages to solve the LP problems.

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This goal led us in the conclusions of (Studený Vomlel Hemmecke 2010) to formulate several research directions (= open mathematical questions). They concern the complexity of a potential future LP procedure for maximization of a quality criterion $\mathcal{Q}$.

Open questions (research directions)

- Get the *outer description* of the polytope P (for any $|N|$).

  The standard version of the simplex method assumes that the region is described in the form of a polyhedron. Therefore, the general characterization of P in this form would be an ideal solution.

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- Describe the *edges* of the polytope P.
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  Because of the above-mentioned interpretation of the simplex method, a potential alternative LP approach may be based only on vertices and edges. Vertices are known, it remains to find edges, which is sometimes easier than finding facets (= outer description).
- Try to apply the geometric approach to *restricted learning* BN structures (e.g. learning undirected trees).
  Learning within a subclass of BN structures is equivalent to maximization over a sub-polytope, which may appear to be simpler!

Recent results: towards outer description

The above mentioned questions were a topic of a conference contribution:

M. Studený and J. Vomlel (2009). On open questions in the geometric approach to learning BN structures. In *Proceedings of WUPES 09* (T. Kroupa, J. Vejnarová eds.), Liblice CZ, September 19-23, 2009.

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Necessary linear constraints:

On the basis of a detailed analysis case of four variables ($|N| = 4$), we have established a class of *necessary linear constraints* on the elements of the polytope P. Specifically, we classified them into three groups:

- the *equality constraints*, denoted by (A),
- *non-specific inequality* constraints, denoted by (B),
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Equality constraints are fully characterized. Their number is $|N| + 1$.
The dimension of the standard imset polytope in $2^{|N|} - |N| - 1$.

Inequality constraints

The observation that the polytope is a part of a formerly studied cone led to a set of *non-specific constraints*. These correspond to the extreme rays of its dual cone (of standardized supermodular functions).

Table: Number of non-specific inequality constraints for $|N| \leq 5$.

$\|N\|$	2	3	4	5
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Specific constraints are in correspondence with certain classes of subsets of N closed under supersets, and, thus, with log-linear models over N.

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Conjecture about the outer description

We proved that all above mentioned inequalities are *necessary* for the points in the polytope P (for any N).

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We would like either confirm or disprove the conjecture for $|N| = 5$ using a computer programm (task for R. Hemmecke and S. Lindner).

Recent results: integral vectors within the polytope

Raymond Hemmecke made earlier some computations for $|N| \leq 5$ to find out whether there exists an imset in the interior of the polytope P and the result was negative.

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Theorem

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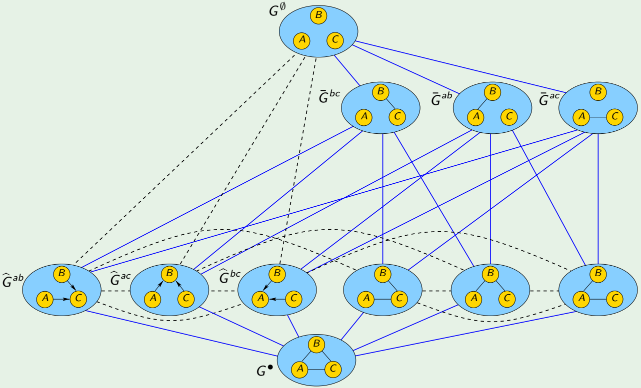
The original proof was quite technical, but it was recently substantially simplified. The idea is to use an elegant linear transformation.

Edges of the standard imset polytope

Example (geometric edges in the case of three variables)



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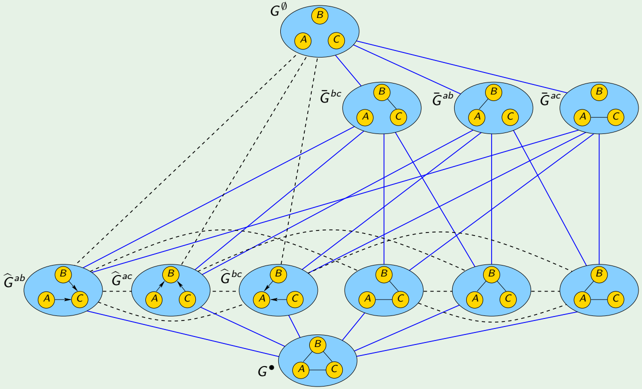

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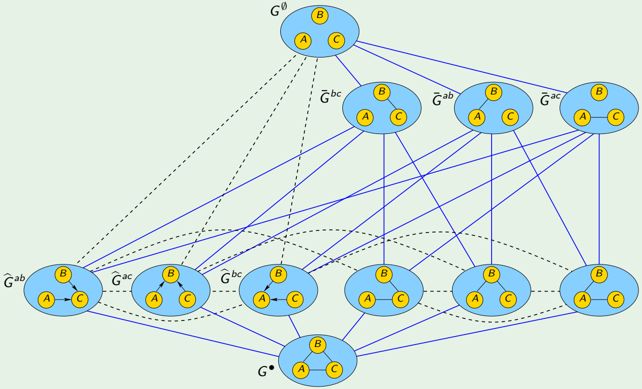

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Nevertheless, what is substantial, are their *directions* (and lengths)!

Recent results: geometric neighborhood

Definition (geometric neighbors, differential imset)

Distinct standard imsets u and v are called *geometric neighbors* if the segment $[u, v]$ is an edge of the polytope. Their difference $w = u - v$ is then called the *differential imset*.

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The result of our analysis in the case $|N| = 4$ was an electronic catalogue of differential imsets for geometric neighbors:

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We have classified their types using three criteria:

- the *squared Euclidean length* of w, i.e. , $\sum_{S \subseteq N} w(S)^2$,
- the number of non-zero imset values, i.e. , $|\{S \subseteq N;\, w(S) \neq 0\}|$, and
- something, which is called the *degree difference* for w.

The idea of restricted learning BN structures

If one considers a subclass of the class of BN structures, then this corresponds to a subset of the set of standard imsets. Geometrically, this subset specifies a sub-polytope of P.

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- the class of BN structures described by acyclic directed graphs with *prescribed order* of nodes (= variables).

Since these subclasses are (sometimes substantially) smaller than the whole class, there is a chance that the corresponding sub-polytope is simpler!

It could be the case the sub-polytope can be characterized in terms of inequalities or in terms of edges, which can result in efficient LP procedures for learning those classes of models.

Restricted learning: forests

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Indeed, the above classic method can be interpreted as a method for maximizing *maximized log-likelihood* (MLL) criterion over *trees*.

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We also plan to have a closer look at the promising linear transformation of standard imsets, which may lead to more intuitive way of geometric description of BN structures.