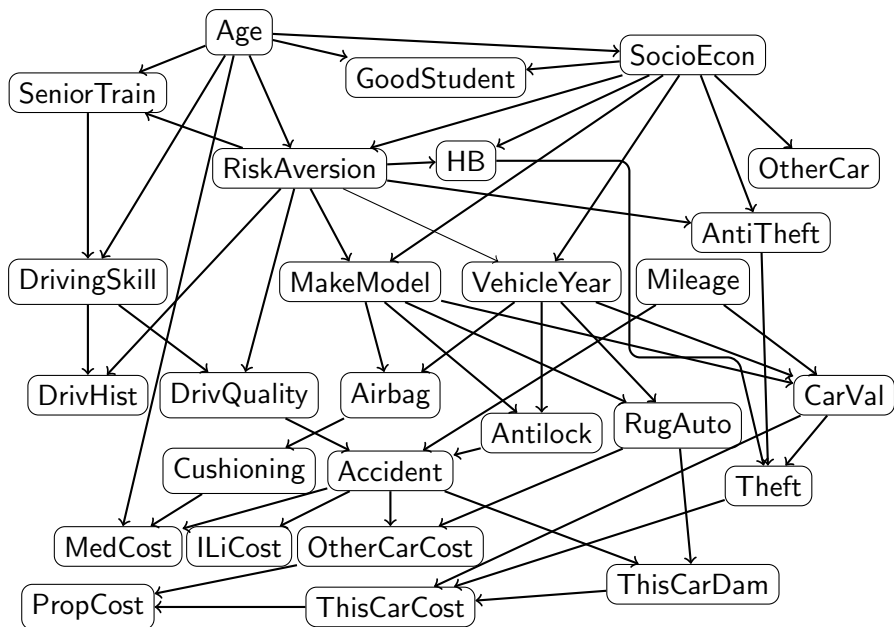


Bayesian network model selection using integer programming

James Cussens, University of York

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The BDeu score

Given complete discrete data D , with an appropriate choice of Dirichlet priors for the parameters, the log marginal likelihood for BN structure G with variables $i = 1, \dots, p$ is:

$$\log P(D|G) = \sum_{i=1}^p c_i(G)$$

where

$$c_i(G) = c_{i \leftarrow \text{Pa}_G(i)} = \sum_{j=1}^{q_i(G)} \left(\log \frac{\Gamma(\alpha_{ij})}{\Gamma(n_{ij} + \alpha_{ij})} + \sum_{k=1}^{r_i} \log \frac{\Gamma(n_{ijk} + \alpha_{ijk})}{\Gamma(\alpha_{ijk})} \right)$$

depends only on the parents variable i has in graph G .

Combinatorial optimisation

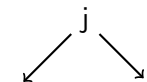
With the preceding assumptions the BN model selection problem is to find a \check{G} such that:

$$\check{G} = \arg \max_G [\log P(D|G)] = \arg \max_G \left[\sum_{i=1}^p c_{i \leftarrow \text{Pa}_G(i)} \right]$$

- ▶ This is a problem of *combinatorial optimisation*,
- ▶ which is known to be NP-hard.

Encoding digraphs as real vectors

- ▶ The key to the integer programming (IP) approach to BN model selection is to view digraphs as points in \mathbb{R}^n .
- ▶ We do this via *family variables*.



- ▶ This digraph: $i \xrightarrow{\quad} k$ is this point in \mathbb{R}^{12} :

$i \leftarrow \{\}$	$i \leftarrow \{j\}$	$i \leftarrow \{k\}$	$i \leftarrow \{j, k\}$
0	1	0	0
$j \leftarrow \{\}$	$j \leftarrow \{i\}$	$j \leftarrow \{k\}$	$j \leftarrow \{i, k\}$
1	0	0	0
$k \leftarrow \{\}$	$k \leftarrow \{i\}$	$k \leftarrow \{j\}$	$k \leftarrow \{i, j\}$
0	0	0	1

BDeu scores as linear objective

Let $x(G)$ be the vector for digraph G , then

$$\log P(D|G) = \sum_{i=1}^p c_{i \leftarrow \text{Pa}_G(i)} = \sum_{i=1}^p \sum_{J: i \notin J} c_{i \leftarrow J} x(G)_{i \leftarrow J}$$

The optimisation problem then becomes: find \check{x} such that

1. $\check{x} = \arg \max cx$
2. \check{x} represents an acyclic digraph

The integer program

We can ensure that x represents an acyclic digraph with two classes of linear constraints and an integrality constraint.

1. 'convexity' $\forall i : \sum_J x_{i \leftarrow J} = 1$
2. 'cluster' $\forall C : \sum_{i \in C} \sum_{J \cap C = \emptyset} x_{i \leftarrow J} \geq 1$
3. x is a zero-one vector

We have an *integer program*: $\max cx$ subject to the above constraints. It is an IP since:

- ▶ the objective function is linear
- ▶ there are only linear and integrality constraints

Relaxation

Solving the following *relaxation* of the problem is very easy

1. $\forall i : \sum_J x_{i \leftarrow J} = 1$
2. ~~$\forall C : \sum_{i \in C} \sum_{J \cap C = \emptyset} x_{i \leftarrow J} \geq 1$~~ (combinatorial relaxation)
3. ~~x is a zero-one vector~~ (linear relaxation)

Relaxations:

- ▶ provide an upper bound on an optimal solution,
- ▶ and we might 'get lucky' and find that the solution to the relaxation satisfies all the constraints of the original problem.

Tightening the relaxation

- ▶ We tighten the relaxation by adding *cutting planes*
- ▶ Let x^* be the solution to the current relaxation,
- ▶ If $\sum_{i \in C} \sum_{J \cap C = \emptyset} x_{i \leftarrow J}^* < 1$ then the valid inequality $\sum_{i \in C} \sum_{J \cap C = \emptyset} x_{i \leftarrow J} \geq 1$ is added to get a new relaxation,
- ▶ and so on.

- ▶ This procedure improves the upper bound.
- ▶ We might get lucky and find that x^* represents an acyclic digraph, in which case the problem is solved.

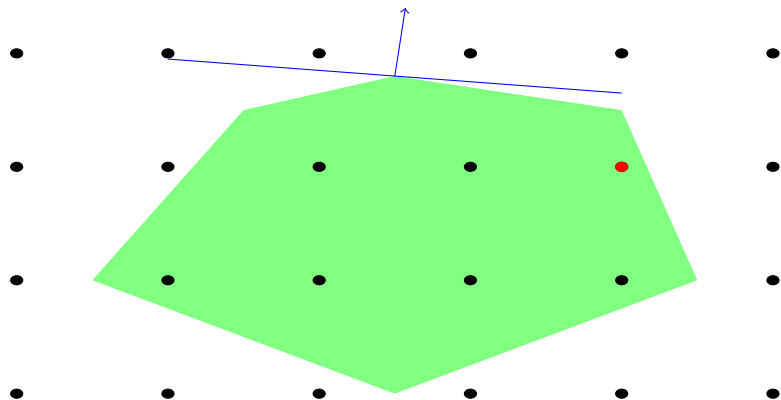
Getting lucky ... eventually

Eskimo pedigree. 1614 BN variables. At most 2 parents. Simulated genotypes. 11934 IP variables.

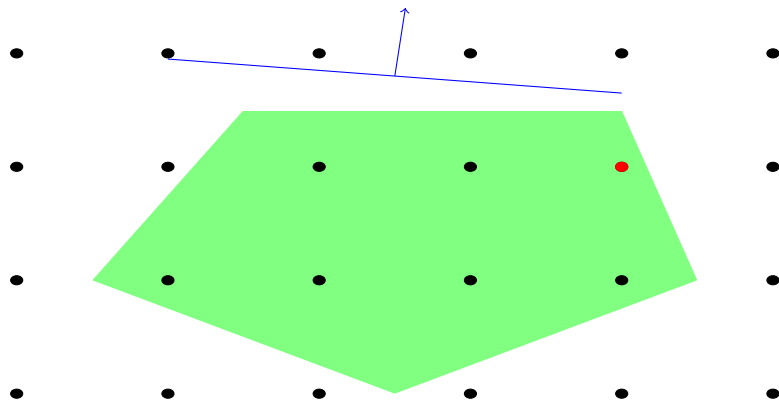
time	frac	cuts	dualbound	primalbound	gap
1110s	120	661	-3.162149e+04	-4.616035e+04	45.98%
1139s	118	669	-3.162175e+04	-4.616035e+04	45.98%
1171s	94	678	-3.162213e+04	-4.616035e+04	45.97%
1209s	26	684	-3.162220e+04	-4.616035e+04	45.97%
1228s	103	685	-3.162223e+04	-4.616035e+04	45.97%
1264s	0	692	-3.162234e+04	-4.616035e+04	45.97%
*1266s	0	-	-3.162234e+04	-3.162234e+04	0.00%

SCIP Status : problem is solved [optimal solution found]
 Solving Time (sec) : 1266.40

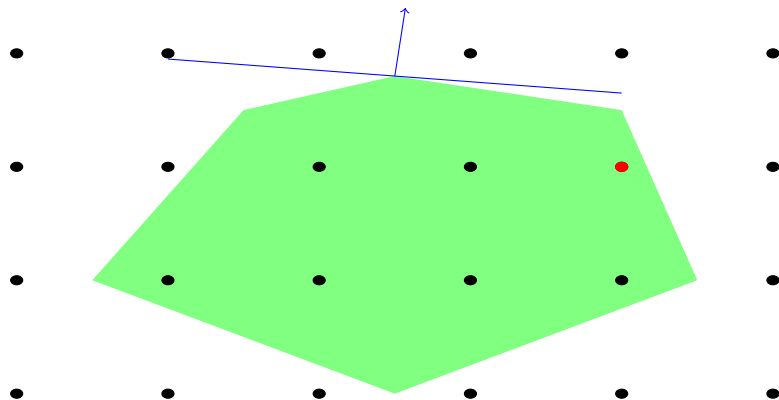
Cutting planes from integrality constraints



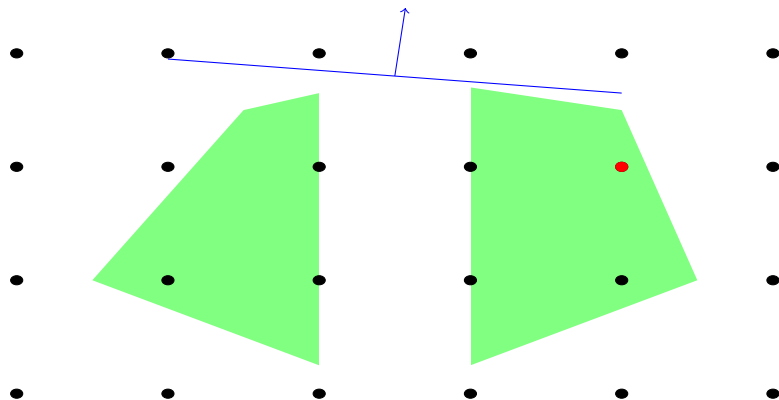
Cutting planes from integrality constraints



Branch-and-bound



Branch-and-bound



Branch and cut

1. Let x^* be the LP solution.
2. If x^* worse than incumbent then exit.
3. If there are valid inequalities
not satisfied by x^*
add them and go to 1.
Else if x^* is integer-valued then
the current problem is solved
Else branch on a variable with
non-integer value in x^*
to create two new sub-problems
(propagate if possible)

The convex hull

- ▶ Since each acyclic digraph is a point in \mathbb{R}^n there is a convex hull of acyclic digraphs.
- ▶ If our IP had all the inequalities defining this convex hull we could drop the integrality restriction and solve the problem with a *linear program* (LP).
- ▶ An LP, unlike, an IP, can be solved in polynomial time.
- ▶ For 4 BN variables, there are 543 acyclic digraphs (living in \mathbb{R}^{28}) and the convex hull is defined by 135 inequalities.

Facets

- ▶ The inequalities defining the convex hull are called *facets*.
- ▶ We have shown [CJKB15, CHS15] that the cluster inequalities, first introduced by [JSGM10], are facets.
- ▶ But there are very many other facets, for example this one for BN variable set $\{a, b, c, d\}$:

$$\begin{aligned}
 & x_{a \leftarrow bc} + x_{a \leftarrow bd} + x_{a \leftarrow cd} + 2x_{a \leftarrow bcd} \\
 & + x_{b \leftarrow ac} + x_{b \leftarrow ad} + x_{b \leftarrow acd} \\
 & + x_{c \leftarrow ab} + x_{c \leftarrow ad} + x_{c \leftarrow abd} \\
 & + x_{d \leftarrow ab} + x_{d \leftarrow ac} + x_{d \leftarrow abc} \leq 2
 \end{aligned}$$

Characteristic imsets and matroids

- ▶ An alternative approach—*characteristic imsets*, developed by Milan Studený—encodes each Markov equivalence class of BNs as a zero-one vector [CHS15].
- ▶ There is a (non-injective) linear map between family-variable vectors and c-imsets.
- ▶ Studený has recently used matroid theory to derive useful results for both the c-imset and family-variable polytope [Stu15].

Limitations





- ▶ Since the BN model selection problem is NP-hard (even with convenient assumptions such as complete data),
- ▶ all methods have to compromise in some way.
- ▶ If the IP solving terminates then we have a BN with guaranteed maximal marginal likelihood,
- ▶ but if we need too many IP variables then we may not get any solution, due to running out of memory.
- ▶ For most problems, it is possible to show that very many family variables will have value zero in any optimal solution—this is what saves us.
- ▶ And/or we can limit the size of parent sets.

Are global optima worth the effort?

- ▶ In a recent paper, Malone *et al* [MJM15] show that “exact approaches, which guarantee to find globally optimal solutions, consistently generalize well to unseen testing data,”
- ▶ In our work using synthetic genetic data, we [SBC14] too found that ‘optimal’ pedigrees were (modestly) more accurate than those found by a heuristic algorithm.

Extensions

- ▶ If we have prior knowledge, such as conditional independence relations, we add these as additional constraints.
- ▶ If the prior on BN structures is 'modular' then we can do MAP model selection (the uniform prior is trivially modular).
- ▶ We can add constraints to rule out *immoralities* to learn decomposable models.
- ▶ Oates *et al* [OSMC15] learned multiple BNs (from multiple datasets) with a penalty for structural differences.

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