Towards the holy grail in machine learning

James Cussens, University of York

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Outline

What is the holy grail in machine learning?

- The user just states:
  1. what they know,
  2. what they want,
  3. and which data they have.
- This is also the goal of *probabilistic programming* (of which more later)
- Claim: CP can help progress towards this holy grail.

The Bayesian approach

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- In the Bayesian approach to machine learning (aka ‘statistical inference’), ‘learning’ is reduced to probabilistic inference.
- Once a prior, likelihood (and perhaps a loss function) has been chosen, this is an entirely deductive process.

Optimisation problems in Bayesian statistics

$$P(M|D) \propto P(M)P(D|M)$$

- The MAP problem: $M^* = \arg\max_M P(M|D)$
- Decision problem: $A^* = \arg\min_A \sum_M L(A,M)P(M|D)$

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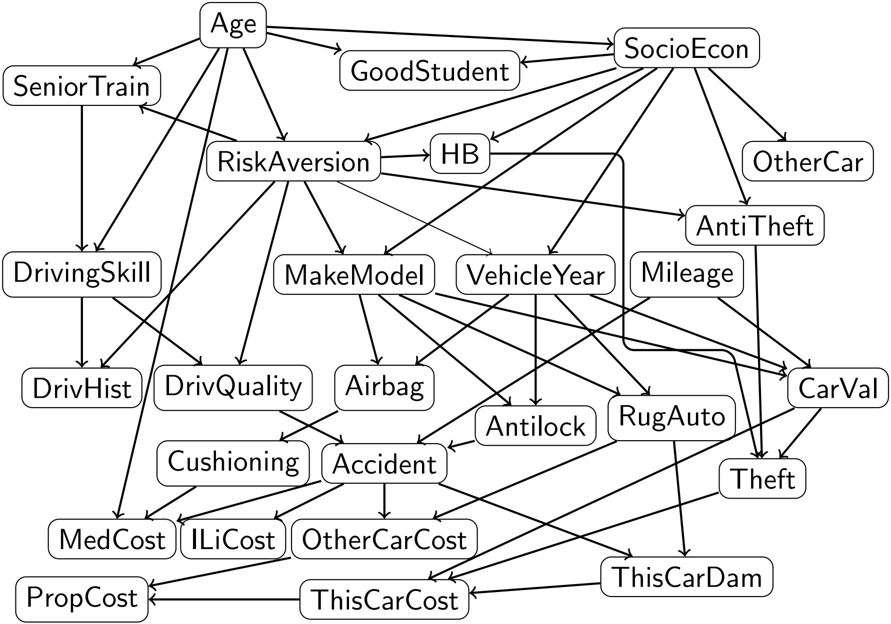
- **NB** The 'optimal' solution depends on our choice of prior.

The holy grail in (Bayesian) machine learning

- Encode all available knowledge/assumptions in the prior and likelihood (and loss function).
- Get some system to find a MAP model, *k*-best models, choose the best action, somehow represent the posterior, whatever.

The role of constraints

- Bayesian inference is easy when the prior is *conjugate*.
- So when estimating the probability of a coin landing heads we typically opt for a Beta distribution, just because it is easier.
- For priors over structures, such as graphs, a uniform distribution is the easy option.
- But in real applications we often have substantive domain knowledge.
- Constraints can be very helpful here.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Antilock
RugAuto
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MedCost
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OtherCarCost
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PropCost
ThisCarCost

Some discrete data

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- From now on write $P(G)$ rather than $P(M)$ to emphasise that the model is a graph.

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 $i = 1, \ldots, p$ is:

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

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

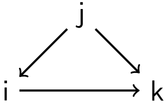
Combinatorial optimisation

With the preceding assumptions the BN model selection problem is to find a G^* such that:

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

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

Encoding graphs as real vectors

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

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

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

The optimisation problem then becomes: find x^* such that

1. $x^* = \arg\max cx$
2. subject to x^* representing an acyclic directed graph.

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- What's the problem here?
- Too many $x(G)_{i \leftarrow J}$ variables!

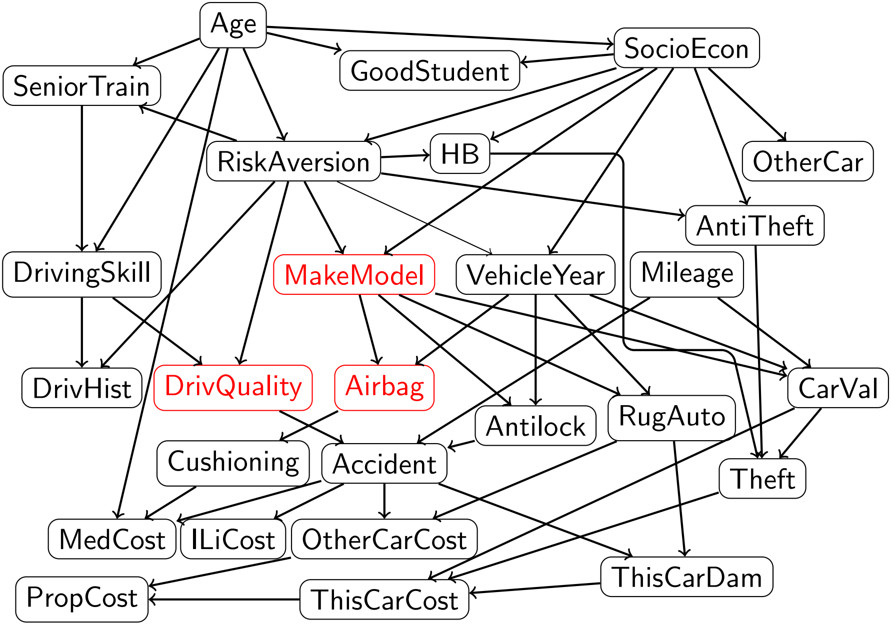
The integer program

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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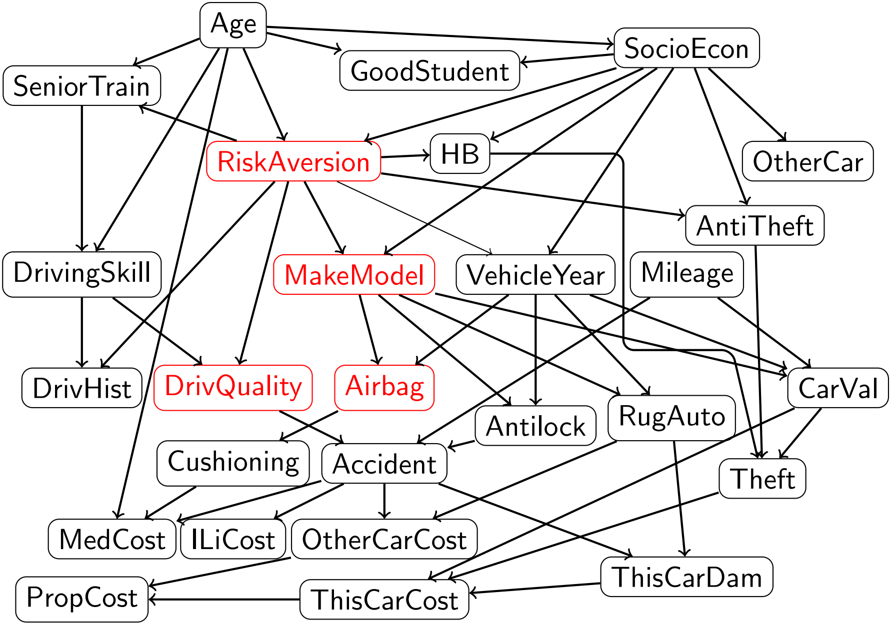
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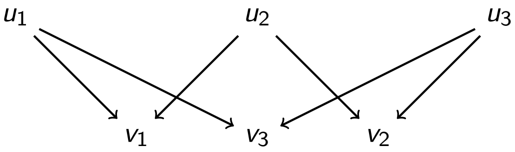
Why IP/CP for BNSL?

- There are very many 'search and score' algorithms for BNSL.
- Hillclimbing is a common choice
- So what are the pros (and cons) of using IP/CP? [Cus11, vBH15]
- A big win is that we can add constraints without needing to come up with a new algorithm.

Necessary constraints in pedigrees

This subgraph can never occur in a DAG representing a *pedigree* ('family tree')



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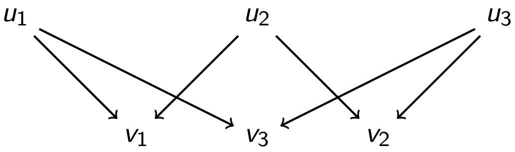

So let, $I_f(u)$ indicate that u is a female, then:
At most one mother:

$$\forall u, v, w : I(\{u, w\} \to v) + I_f(u) + I_f(w) \leq 2$$

At least one mother:

$$\forall u, v, w : I(\{u, w\} \to v) - I_f(u) - I_f(w) \leq 0$$

Digression: Exploiting the solver

- I'm advocating a *declarative approach* to machine learning: declare what we know and leave the rest to the solver.
- A nice plus: many IP solvers (CPLEX, Gurobi and SCIP) allow you to find:
  - the k-best solutions
  - all solutions with objective value above some threshold
- If getting an optimal solution is impractical, you at least get an optimality gap.
- Moreover, CPLEX and Gurobi (and SCIP using UG) will grab available cores with zero effort from the user.

Other constraints for BNSL

1. There must (not) be an arrow from A to B
2. There must (not) be a path from A to B
3. If A and B are co-parents there must be an edge between them (chordality).
4. The graph must satisfy certain conditional independence relations.

- All easy to throw in.

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- All easy to throw in.
- But not always easy to ensure fast solving!

Why 'cluster' constraints?

$$\forall C : \sum_{i \in C} \sum_{J \cap C = \emptyset} x_{i \leftarrow J} \geq 1$$

- One can rule out cycles in graphs with a quadratic number of linear constraints (and a linear number of additional variables).
- We choose to use exponentially many cluster constraints [JSGM10] since they are *facets* of the convex hull of directed acyclic graphs, leading to a tight linear relaxation.
- They are added as *cutting planes* 'on the fly'. (Finding one is NP-hard; a sub-IP is used.)
- Studený [Stu15] showed that there is a facet associated with every *connected matroid*. Cluster constraints are a special case.

Not all facets are equal

- We computed all the 135 facets of the convex hull of the 543 DAGs when there are only 4 BN variables. Ones like this improved performance far more than others. Why?

$$
\begin{aligned}
& x_{a\leftarrow\{b,c\}} + x_{a\leftarrow\{b,d\}} + x_{a\leftarrow\{b,c,d\}} + \\
& x_{b\leftarrow\{a,c\}} + x_{b\leftarrow\{a,d\}} + x_{b\leftarrow\{a,c,d\}} + \\
& x_{c\leftarrow\{d\}} + x_{c\leftarrow\{a,b\}} + x_{c\leftarrow\{a,d\}} + x_{c\leftarrow\{b,d\}} + x_{c\leftarrow\{a,b,d\}} + \\
& x_{d\leftarrow\{c\}} + x_{d\leftarrow\{a,b\}} + x_{d\leftarrow\{a,c\}} + x_{d\leftarrow\{b,c\}} + x_{d\leftarrow\{a,b,c\}} \leq 2
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\end{aligned}
$$

- This facet is *score-equivalent*. If two BNs are Markov equivalent then the LHS of the facet is the same for both BNs.
- And we typically use objectives that are score-equivalent.
- The facet above corresponds to the (connected) matroid whose *circuits* are $\{\{a,b,c\},\{a,b,d\},\{c,d\}\}$.

The too-many variables problem

- Problem: We can only fit so many $x_{i \leftarrow J}$ family variables into the solver.
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- 'Pruning' is used to delete many, but we can still end up with too many.
- Very few $x_{i \leftarrow J}$ family variables have non-zero value in any solution.
- Solution: Create IP variables on the fly using a *pricer*.
- This is the dual of adding cutting planes ('constraints on the fly').
- The implementation requires a lot of bookkeeping :-(

An alternative approach to BNSL

- I have just presented a *search and score* approach to BNSL.
- The other main approach is known as *constraint-based* BN learning.
- (There are also hybrid approaches.)

Constraint-based BN learning

- A Bayesian network encodes a set of *conditional independence relations*.
- Is A independent of B given C? ($A \perp B|C$?)
- So ask which conditional independence relations hold and which do not and then view the answers as *constraints* on an acceptable DAG.
- It may be that only a DAG with *latent* (i.e. unobserved) and/or *selection* (i.e. conditioned on) variables satisfies all the constraints.
- Either use statistical tests on the data or pretend we have an oracle to answer these questions.
- For efficiency only do some tests.

CP for Constraint-based BN learning

- Constraint-based BN learning is a *constraint satisfaction* problem, . . .
- . . . albeit one where not all constraints are known at the outset.
- However the best-known algorithms for constraint-based BN learning (PC, FCI, RFCI) do not use CP methods.
- But CP based methods do exist: *Constraint-based Causal Discovery: Conflict Resolution with Answer Set Programming* [HEJ14]

Probabilistic Programming

From the Stan website:

"Users specify log density functions in Stan's probabilistic programming language and get:

- full Bayesian statistical inference with MCMC sampling (NUTS, HMC)
- approximate Bayesian inference with variational inference (ADVI)
- penalized maximum likelihood estimation with optimization (L-BFGS)"

The (log) density function is typically a posterior distribution.

Is Stan declarative or imperative?

"A Stan program defines a statistical model through a conditional probability function $p(\theta|y, x)$, where θ is a sequence of modeled unknown values (e.g., model parameters, latent variables, missing data, future predictions),
Stan is an imperative language, like C or Fortran (and parts of C++, R, Python, and Java), in the sense that is based on assignment, loops, conditionals, local variables, object-level function application, and array-like data structures."

Constrained optimisation in Machine Learning

- Constrained optimisation is everywhere in Machine Learning.
- For example, using Support Vector Machines involves solving a quadratic programming problem (which is typically not solved by sending the problem to a QP solver).
- Sometimes CP methods explicitly used, particularly for: clustering, frequent item-set mining, BNSL/causal inference.
- See the AIJ Special Issue [PTG17] for example.

MiningZinc: A Language for Constraint-based Mining

- "MiningZinc is a high-level language for constraint-based mining that supports both user-defined constraints and efficient, specialised solving. It consists of a language and a framework."
- Can be applied to e.g. frequent itemset mining and clustering.
- "The language is standard MiniZinc."
- "It supports both generic CP, SAT and MIP solvers, as well as specialised constraint-based mining systems."

Constraints and the democratisation of machine learning

- If we can simply declare what the learning task is, can the process of machine learning be automated (and de-skilled)?
- Consider the SYNTH project: "What we want to do in the SYNTH project is to automate a subfield of AI itself. That field is data science, ..."
- Will the end-user understand what has happened?
- Need to distinguish how to optimise (computational) from what to optimise (statistical).

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