Towards the holy grail in machine learning

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Outline

The holy grail

The Bayesian approach

Bayesian network learning

Probabilistic Programming

CP in Machine Learning
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

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.

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P(M|D) \propto P(M)P(D|M) = P(M) \int_\theta P(D|M, \theta)P(\theta)d\theta
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The Bayesian approach

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The Bayesian approach

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: \( A^* = \arg\min_A \sum_M L(A, M)P(M|D) \)

The 'optimal' solution depends on our choice of prior.
The Bayesian approach

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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 Bayesian approach

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.
Bayesian network learning

Some discrete data

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....
A Bayesian approach

\[ P(M|D) \propto P(M) \int_{\theta} P(D|M, \theta)P(\theta)d\theta \]

- Choose (for the time being) a uniform prior for \( P(M) \)
- Choose the \( P(\theta) \) so the integral (the marginal likelihood) has a closed form
A Bayesian approach

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- Choose (for the time being) a uniform prior for \( P(M) \)
- Choose the \( P(\theta) \) so the integral (the marginal likelihood) has a closed form
- 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:

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

where $c_i(G)$, the local score for variable $i$ depends only on the parents variable $i$ has in graph $G$. 
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$$c_i(G) = c_{i \leftarrow Pa_G(i)} = \sum_{j=1}^{q_i(G)} \left( \log \frac{\Gamma(\alpha_{ij})}{\Gamma(n_{ij} + \alpha_{ij})} + \sum_{k=1}^{r_i} \log \frac{\Gamma(n_{ijk} + \alpha_{ijk})}{\Gamma(\alpha_{ijk})} \right)$$
With the preceding assumptions the BN model selection problem is to find a $G^*$ such that:

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

- This is a problem of *combinatorial optimisation*,
- which is known to be NP-hard.
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: $i \xrightarrow{} j \xrightarrow{} k$ is this point in $\mathbb{R}^{12}$:

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

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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’ $\forall i : \sum_{J \ni J} x_{i \leftarrow J} = 1$
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
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’)

![Diagram](image)

If \( u \) indicate that \( u \) is a female, then:

At most one mother:

\[
\forall u, v, w: I(u \{u, w\} \rightarrow v) + I(f(u)) + I(f(w)) \leq 2
\]

At least one mother:

\[
\forall u, v, w: I(u \{u, w\} \rightarrow v) - I(f(u)) - I(f(w)) \leq 0
\]
Necessary constraints in pedigrees

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

\[ u_1 \rightarrow v_1 \rightarrow u_2 \rightarrow v_2 \rightarrow u_3 \rightarrow v_3 \]

So let, \( l_f(u) \) indicate that \( u \) is a female, then:

At most one mother:
\[
\forall u, v, w : l(\{u, w\} \rightarrow v) + l_f(u) + l_f(w) \leq 2
\]

At least one mother:
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\forall u, v, w : l(\{u, w\} \rightarrow v) - l_f(u) - l_f(w) \leq 0
\]
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.
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?

\[ \begin{align*}
  x_{a \leftarrow \{b,c\}} &+ x_{a \leftarrow \{b,d\}} + x_{a \leftarrow \{b,c,d\}} + \\
  x_{b \leftarrow \{a,c\}} &+ x_{b \leftarrow \{a,d\}} + x_{b \leftarrow \{a,c,d\}} + \\
  x_{c \leftarrow \{d\}} &+ x_{c \leftarrow \{a,b\}} + x_{c \leftarrow \{a,d\}} + x_{c \leftarrow \{b,d\}} + x_{c \leftarrow \{a,b,d\}} + \\
  x_{d \leftarrow \{c\}} &+ x_{d \leftarrow \{a,b\}} + x_{d \leftarrow \{a,c\}} + x_{d \leftarrow \{b,c\}} + x_{d \leftarrow \{a,b,c\}} \leq 2
\end{align*} \]
Not all facets are equal

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\[
X_{a \leftarrow \{b, c\}} + X_{a \leftarrow \{b, d\}} + X_{a \leftarrow \{b, c, d\}} + \\
X_{b \leftarrow \{a, c\}} + X_{b \leftarrow \{a, d\}} + X_{b \leftarrow \{a, c, d\}} + \\
X_{c \leftarrow \{d\}} + X_{c \leftarrow \{a, b\}} + X_{c \leftarrow \{a, d\}} + X_{c \leftarrow \{b, d\}} + X_{c \leftarrow \{a, b, d\}} + \\
X_{d \leftarrow \{c\}} + X_{d \leftarrow \{a, b\}} + X_{d \leftarrow \{a, c\}} + X_{d \leftarrow \{b, c\}} + X_{d \leftarrow \{a, b, c\}} \leq 2
\]

- 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.

‘Pruning’ is used to delete many, but we can still end up with too many.
The too-many variables problem

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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.)
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.
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]
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 $\theta$ 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 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 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.”
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).
James Cussens.
Bayesian network learning with cutting planes.

A. Hyttinen, F. Eberhardt, and M. Järvisalo.
Constraint-based causal discovery: Conflict resolution with answer set programming.

Tommi Jaakkola, David Sontag, Amir Globerson, and Marina Meila.
Learning Bayesian network structure using LP relaxations.
Andrea Passerini, Guido Tack, and Tias Guns.  
Special issue on combining constraint solving with mining and learning.  

Milan Studený.  
How matroids occur in the context of learning Bayesian network structure.  

Peter van Beek and Hella-Franziska Hoffmann.  
Machine learning of Bayesian networks using constraint programming.  
In *Proc. CP 2015*, August 2015.