Imprecise Probabilities in AI

Bayesian networks

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Initial setup

- Four binary variables:
  - $X_1 \in \{true, false\}$: High temperature
  - $X_2 \in \{true, false\}$: Goalkeeper's fitness
  - $X_3 \in \{true, false\}$: Attackers' fitness
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- We can build this function from data, constraints, experts, etc.
  - This is usually called *learning* in the context of prob graphical models (PGMs).
- We can use $P(X_1, X_2, X_3, X_4)$ (somehow encoded into bits) to compute queries such as $P(X_1 = true | X_4 = true)$ or $\arg\max_{X_4} P(X_4 | X_1 = false)$.
  - This is usually called *reasoning/inferences* in the context of PGMs.

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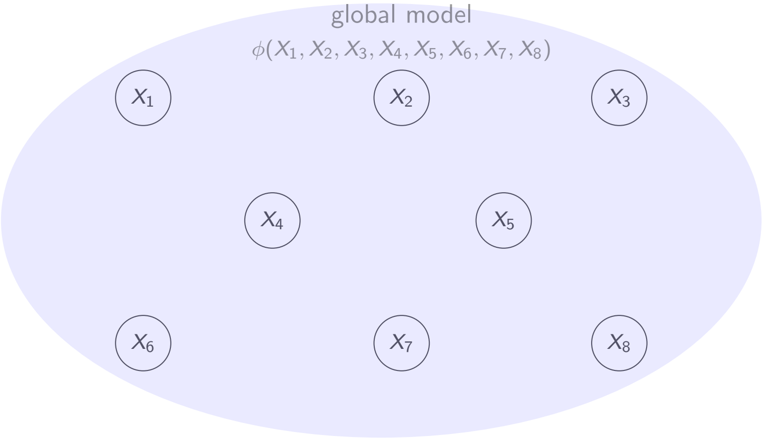
- **Q:** Aren't these all "trivial" tasks? **A:** If you have a (potentially huge) table representing $P(\mathbf{X})$, then yes: just go over the table.

Probabilistic Graphical Models

aka Decomposable Multivariate Probabilistic Models

(whose decomposability is induced by independence)



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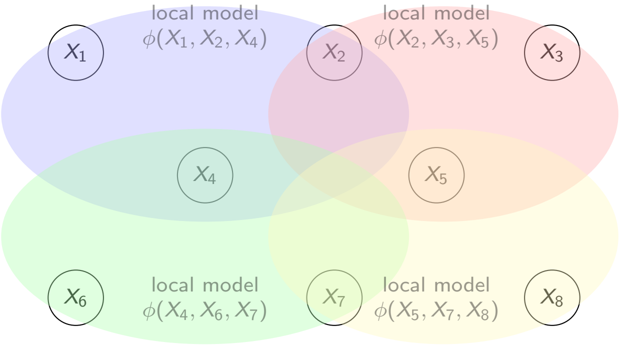
$$\phi(X_1, X_2, X_3, X_4, X_5, X_6, X_7, X_8) = \phi(X_1, X_2, X_4) \otimes \phi(X_2, X_3, X_5) \otimes \phi(X_4, X_6, X_7) \otimes \phi(X_5, X_7, X_8)$$



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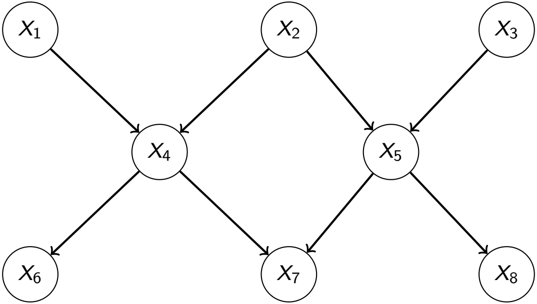
directed graphs

Bayesian/credal networks

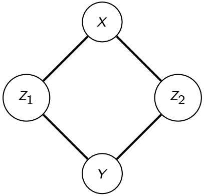


Markov Condition

- Probabilistic model over set of variables $(X_1, \ldots, X_n)$ in one-to-one correspondence with the nodes of a graph

Undirected Graphs

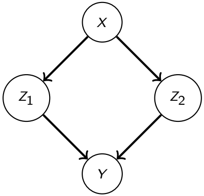
X and Y are independent given Z
if any path between X and Y
containts an element of Z



Directed Graphs

Given its parents, every node is independent of its (non-parent) non-descendants

X and Y are d-separated by Z if, along every path between X and Y there is a W such that either W has converging arrows and is not in Z and none of its descendants are in Z, or W has no converging arrows and is in Z



Directed Graphs

We choose to discuss further on directed graphs here. Some reasons:

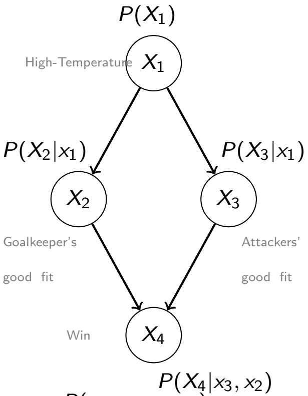
- Normalised distributions help with interpretability of local models.
- Directed edges help with sampling.
- Directed edges can be used for causal inference.
- Representation power (a.k.a. expressivity) is similar to undirected models.
- Computational costs are similar to undirected models.

(The Markov condition is arguably harder to describe/interpret than with its undirected counterpart.)

Bayesian networks

- Set of categorical variables $X_1, \ldots, X_n$
- Directed acyclic graph
  - conditional (stochastic) independencies according to the Markov condition:

    "any node is conditionally independent of its non-descendents given its parents"
- A conditional mass function for each node and each possible value of the parents
  - $\{P(X_i|\mathrm{pa}(X_i)),\ \forall i = 1, \ldots, n,\ \forall \mathrm{pa}(X_i)\}$
- Defines a joint probability mass function
  - $P(x_1, \ldots, x_n) = \prod_{i=1}^{n} P(x_i|\mathrm{pa}(X_i))$



$P(x_1, x_2, x_3, x_4) =$
$P(x_1)P(x_2|x_1)P(x_3|x_1)P(x_4|x_3, x_2)$

E.g., given temperature, fitnesses independent

Bayesian network - simple example - bn1.txt

```
library(bnlearn)
source('my.bn.inference.r')
net = model2network("[x1][x2|x1][x3|x1][x4|x2:x3]")

cpt1.x1 = matrix(c(0.7, 0.3), ncol = 2,
    dimnames = list(NULL, c('true', 'false')))
cpt1.x2 = c(0.1, 0.9, 0.3, 0.7)
dim(cpt1.x2) = c(2, 2)
dimnames(cpt1.x2) = list("x2" = c("true", "false"),
            "x1" =  c("true", "false"))
cpt1.x3 = c(0.5, 0.5, 0.2, 0.8)
dim(cpt1.x3) = c(2, 2)
dimnames(cpt1.x3) = list("x3" = c("true", "false"),
            "x1" =  c("true", "false"))
cpt1.x4 = c(0.9, 0.1, 0.5, 0.5, 0.4, 0.6, 0.1, 0.9)
dim(cpt1.x4) = c(2, 2, 2)
dimnames(cpt1.x4) = list("x4" = c("true", "false"),
            "x2" =  c("true", "false"),
            "x3" = c("true", "false"))
```

Bayesian network - simple example - bn2.txt

```
net.1 = custom.fit(net, dist = list(x1=cpt1.x1,
                             x2=cpt1.x2, x3=cpt1.x3, x4=cpt1.x4))

query=rep(NA,length(net.1))
names(query) <- names(net.1)
query[2]='false'
my.bn.inference(net.1,query)
## $logp.evi
## [1] 0
## $logp.query
## [1] -0.1743534
## $p
## [1] 0.84
## $evidence
## [1] ""
## $query
## [1] "x2=false"
```

Bayesian network - simple example - bn3.txt

```
query[1]='true'
my.bn.inference(net.1,query)
## $logp.evi
## x[1] 0
## $logp.query
## [1] -0.4620355
## $p
## [1] 0.63
## $evidence
## [1] ""
## $query
## [1] "x1=true,x2=false"
```

Bayesian network - simple example - bn4.txt

```
evidence=rep(NA,length(net.1))
names(evidence) <- names(net.1)
evidence[4]='true'
res <- my.bn.inference(net.1,query,evidence)
##res not shown
evidence[4]='false'
my.bn.inference(net.1,query,evidence)
## $logp.evi
## [1] -0.3816998
## $logp.query
## [1] -0.8187104
## $p
## [1] 0.6459646
## $evidence
## [1] "x4=false"
## $query
## [1] "x1=true,x2=false"
```

Bayesian network - simple example - bn5.txt

```
my.bn.inference(net.1,NA,NA,map.query=TRUE)
## $logp.evi
## [1] -1.260543
## $p
## [1] 0.2835
## $map
##      x1   x2    x3    x4
## 16 true false false false
## $evidence
## [1] ""
evidence
##     x1      x2      x3      x4
##     NA      NA      NA "false"
my.bn.inference(net.1,NA,evidence,map.query=TRUE)
evidence[4]='true'
my.bn.inference(net.1,NA,evidence,map.query=TRUE)
```

Reasoning with Bayesian networks

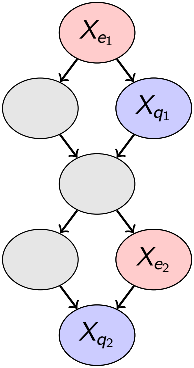
- Conditional probs for a variable of interest X_q given observations $X_E = x_E$

$$P(x_q|x_E) = \frac{P(x_q, x_E)}{P(x_E)} = \frac{\sum_{\mathbf{x}\setminus\{x_q,x_E\}} \prod_{i=1}^n P(x_i|\pi_i)}{\sum_{\mathbf{x}\setminus\{x_E\}} \prod_{i=1}^n P(x_i|\pi_i)}$$

- MAP/MPE queries can be even harder

$$\max_{\mathbf{x}_Q} P(\mathbf{x}_Q, \mathbf{x}_E) = \max_{\mathbf{x}_Q} \sum_{\mathbf{x}\setminus\{\mathbf{x}_Q,\mathbf{x}_E\}} \prod_{i=1}^n P(x_i|\pi_i)$$

- Updating Bayesian nets is NP-hard
(fast algorithms for belief updating and full MPE in polytree/bounded treewidth nets)



Bayesian network structures

Graph structures induce different factorisations. Examples:

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- $P(X_1, X_2, X_3, X_4) = P(X_1|X_2, X_3, X_4)P(X_2|X_3, X_4)P(X_3|X_4)P(X_4)$

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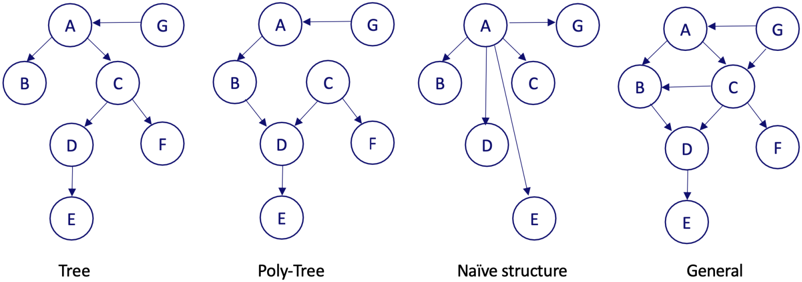
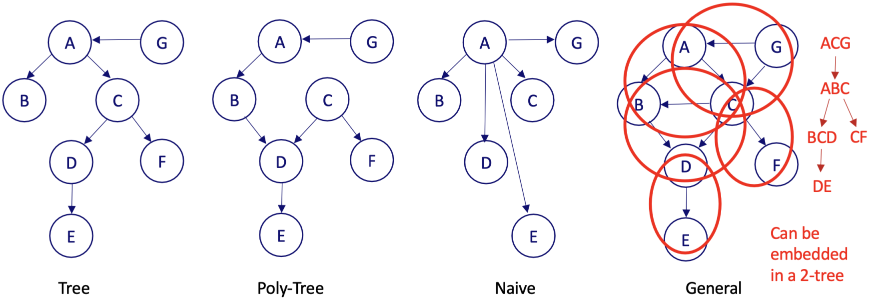
- ...

Key fact: model size grows linearly in the number of variables if local conditional functions are bounded (i.e. not so many parents per node).

Bayesian network structure complexity



Bayesian network tree-width



Minimum treewidth: how small is the k to which we can embed the moralised graph of a Bayesian net in a k-tree graph (roughly a hyper-tree where each node is contained in a (k+1)-clique).

Learning Bayesian networks

Two main approaches to structure learning:

- Find the graph structure with highest score. Possible scores:
  - Max. Likelihood (break ties towards simplicity)
  - Bayesian Dirichlet (Equivalent Uniform)
  - Bayesian Information Criterion
  - Minimum Description Length
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Parameter learning usually done with standard estimators:

- (Penalised) Maximum likelihood
- Bayesian updating (multinomial Dirichlet)

Some references

- Koller, D. and Friedman, N. (2009). *Probabilistic Graphical Models*. MIT Press.
- Darwiche, A. (2009). *Modeling and Reasoning with Bayesian Networks* Cambridge Press.
- Pearl, J. (1988). *Probabilistic reasoning in intelligent systems: networks of plausible inference*. Morgan Kaufmann.