732A96/TDDE15 Advanced Machine Learning

Graphical Models

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Lecture 4: Structure Learning

Contents

Literature

- Main source
  - Koski, T. J. T. and Noble, J. M. A Review of Bayesian Networks and Structure Learning. *Mathematica Applicanda* 40, 51-103, 2012.

Structure Learning for BNs: Independence Test Based Approach

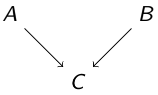
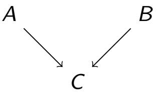
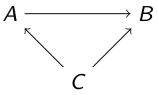
- We can get a DAG G to be used for **probabilistic** reasoning as follows:

Let $Y_{1:n}$ be any ordering of the random variables $X_{1:n}$
For each Y_i do
    Set Pa_i to be any minimal subset of $Y_{1:i-1}$ such that $Y_i \perp_p Y_{1:i-1} \setminus Pa_i | Pa_i$

- **Exercise**. Prove the previous statement.

Structure Learning for BNs: Independence Test Based Approach

- Note that G has the minimum number of edges among the DAGs that are consistent with the ordering considered.
- However, G may not have the minimum number of edges among all the DAGs, i.e. the ordering considered may not be optimal.

$A \perp_p B$	G with ordering A, B, C	G with ordering C, A, B
		

- Since the ordering of the variables in the construction of the DAG is arbitrary, we cannot interpret the DAG as a causal structure and, thus, we should not use it for **causal** reasoning.
- As we will see next, we can get a DAG with minimum number of edges without searching over the $n!$ orderings assuming that p is **faithful** to the true DAG G^*, i.e. $U \perp_p V | Z$ if and only if $U \perp_{G^*} V | Z$. Yet the DAG learned should **only** be used for probabilistic reasoning.

Structure Learning for BNs: Independence Test Based Approach

Parents and children (PC) algorithm

Let G be the complete undirected graph
Let $Ad(X_i)$ denote the nodes adjacent (i.e., linked) to X_i in G
$l := 0$
Repeat while $l \leq n - 2$
    For each ordered pair of nodes X_i and X_j in G such that $X_i \in Ad(X_j)$ and $|Ad(X_i) \setminus X_j| \geq l$
        If there is some $S \subseteq Ad(X_i) \setminus X_j$ such that $|S| = l$ and $X_i \perp_p X_j | S$, then
            $S_{ij} := S_{ji} := S$
            Remove the edge $X_i - X_j$ from G
    $l := l + 1$
Apply the rule R1 to G while possible
Apply the rules R2-R4 to G while possible

R1: $X_i \text{ --- } X_j \text{ --- } X_k \wedge X_j \notin S_{ik} \quad \Rightarrow \quad X_i \longrightarrow X_j \longleftarrow X_k$

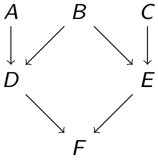
R2: $X_i \longrightarrow X_j \text{ --- } X_k \quad \Rightarrow \quad X_i \longrightarrow X_j \longrightarrow X_k$

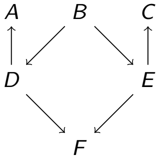
R3:
$$\begin{tikzcd} X_i \arrow[r] \arrow[rr, dash, bend left] & X_j \arrow[r] & X_k \end{tikzcd} \quad \Rightarrow \quad \begin{tikzcd} X_i \arrow[r] \arrow[rr, bend left] & X_j \arrow[r] & X_k \end{tikzcd}$$

R4:
$$\begin{tikzcd} & X_k \arrow[dr] & \\ X_i \arrow[ur, dash] \arrow[rr, dash] \arrow[dr, dash] & & X_j \\ & X_l \arrow[ur] & \end{tikzcd} \quad \Rightarrow \quad \begin{tikzcd} & X_k \arrow[dr] & \\ X_i \arrow[ur, dash] \arrow[rr] \arrow[dr, dash] & & X_j \\ & X_l \arrow[ur] & \end{tikzcd}$$

Structure Learning for BNs: Independence Test Based Approach

- **Exercise**. Run the PC algorithm assuming that p is faithful to the following DAGs.





Structure Learning for BNs: Independence Test Based Approach

- In practice, we do not have access to p but to a finite sample from it. Then, replace $X_i \perp_p X_j | S$ in the PC algorithm with an independece test, preferably with one that is consistent so that the algorithm is **asymptotically** correct.
- Let $d_{1:N}$ be a complete sample. Then, $X_i \perp_p X_j | S$ implies that $p(x_i, x_j | s) = p(x_i | s) p(x_j | s)$ and thus that

$$N_{x_i, x_j, s} \approx N_{x_i, s} N_{x_j, s} / N_s$$

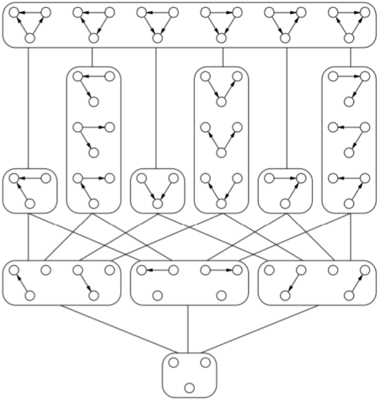
  where $N_{x_i, x_j, s}$ is the number of instances in $d_{1:N}$ where x_i, x_j and s, and $N_{x_i, s} = \sum_{x_j} N_{x_i, x_j, s}$ and $N_{x_j, s} = \sum_{x_i} N_{x_i, x_j, s}$ and $N_s = \sum_{x_i, x_j} N_{x_i, x_j, s}$.
- We can measure the deviance from the expected situation above by

$$deviance = \sum_{x_i, x_j, s} \frac{[N_{x_i, x_j, s} - N_{x_i, s} N_{x_j, s} / N_s]^2}{N_{x_i, s} N_{x_j, s} / N_s}$$

- If the deviance is too large, then reject the hypothesis that $X_i \perp_p X_j | S$.
- Asymptotically, the deviance follows a χ^2 distribution with the appropriate number of degrees of freedom, i.e. $|S|(|X_i| - 1)(|X_j| - 1)$. Then, we can control the probability of falsely rejecting the hypothesis, a.k.a. p-value.

Structure Learning for BNs: Independence Test Based Approach

- Two DAGs represent the same independencies according to the separation criterion (i.e. they are **equivalent**) if and only if they have the same adjacencies and **unshielded colliders**, i.e. subgraphs $X_i \rightarrow X_k \leftarrow X_j$ where X_i and X_j are not adjacent.



Hasse diagram of the space of Markov equivalence classes of Bayesian network structures over three variables.

Structure Learning for BNs: Independence Test Based Approach

- The output of the PC algorithm is not a DAG in general, but an **essential graph** (EG):
  - The EG G has an edge $X_i \rightarrow X_j$ if and only if $X_i \rightarrow X_j$ is in **every** DAG that is equivalent to the true DAG G^*.
  - In other words, G has an edge $X_i - X_j$ if and only if $X_i \rightarrow X_j$ is in some DAG that is equivalent to G^* and $X_i \leftarrow X_j$ is in some other DAG that is equivalent to G^*.
- A naive way to convert G into a DAG that is equivalent to G^* is as follows:

Repeat while possible

  Replace any edge $X_i - X_j$ in G with $X_i \rightarrow X_j$ if this does not create a directed cycle or a new unshielded collider

If G is not a DAG, then backtrack

- Again, G can be used for probabilistic reasoning but not for causal reasoning.

Structure Learning for BNs: Score Based Approach

- Alternatively, we can choose the DAG G with maximum posterior probability (a.k.a **Bayesian score**):

$$p(G|d_{1:N}) = p(d_{1:N}|G)p(G)/P(d_{1:N}) \propto p(d_{1:N}|G)p(G)$$

  where $p(d_{1:N}|G)$ is the marginal likelihood of $d_{1:N}$ given G, $p(G)$ is a prior probability distribution, and $p(d_{1:N})$ is a normalization constant.

- Moreover

$$p(d_{1:N}|G) = \int p(d_{1:N}|\theta, G)p(\theta|G)d\theta$$

  where $p(d_{1:N}|\theta, G)$ is the likelihood function of $d_{1:N}$ given G and θ, and $p(\theta|G)$ is a prior probability distribution.

- **Assuming** that $p(\theta|G) = \prod_i \prod_j p(\theta_{x_i|Pa_i=j}|G)$ and $p(\theta_{x_i|Pa_i=j}|G) \sim Dirichlet(\alpha_{ij1}, \ldots, \alpha_{ijk_i})$, we have that

$$p(d_{1:N}|G) = \prod_i \prod_j \frac{\Gamma(\alpha_{ij})}{\Gamma(\alpha_{ij} + N_{ij})} \prod_k \frac{\Gamma(\alpha_{ijk} + N_{ijk})}{\Gamma(\alpha_{ijk})}$$

  where $\alpha_{ij} = \sum_k \alpha_{ijk}$, N_{ijk} is the number of instances in $d_{1:N}$ where $X_i = k$ and $Pa_i = j$, and $N_{ij} = \sum_k N_{ijk}$.

Structure Learning for BNs: Score Based Approach

- The Bayesian score is **score equivalent** (i.e. it gives the same score to equivalent DAGs) if
$$\alpha_{ijk} = \frac{\alpha}{|X_i| \prod_{X_l \in Pa_i} |X_l|}$$
where α is the user-defined imaginary sample size (the higher the less regularization). This is call the BDeu score.
- Under the Dirichlet parameter prior assumption and when $N \to \infty$, we have that
$$\log p(d_{1:N}|G) \approx \log p(d_{1:N}|\theta^{ML}, G) - \frac{\log N}{2} dim(G)$$
where $dim(G)$ is the dimension or number of free parameters of G, i.e. $\sum_i (|X_i| - 1) \prod_{X_l \in Pa_i} |X_l|$.
- This approximation is called **Bayesian information criterion** (BIC), and it shows that the Bayesian score favours models that trade off fit of data and model complexity.

Structure Learning for BNs: Score Based Approach

- Number of DAGs with 1-12 nodes: 1, 3, 25, 543, 29281, 3781503, 1138779265, 783702329343, 1213442454842881, 4175098976430598143, 31603459396418917607425, 521939651343829405020504063
- Then, an exhaustive search is prohibitive. Then, a heuristic search must be performed instead.

Hill-climbing (HC)

Let G be the empty DAG
Repeat until no change occurs
    Add, remove or reverse any edge in G that improves the Bayesian score the most

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- Unlike the PC algorithm, HC is not asymptotically correct under faithfulness, i.e. it may get trapped in local optima. Still, HC is very popular.

Structure Learning for MNs: Independence Test Based Approach

- We can get an UG G to be used for probabilistic reasoning as follows:

For each X_i do
  Set $Ad(X_i)$ to be any minimal subset of $X \setminus X_i$ such that $X_i \perp_p X \setminus Ad(X_i) | Ad(X_i)$

- Luckily, we can get G without searching over the 2^{n-1} possible adjacent sets for each node if we assume that p is **faithful** to the true MN G^*, i.e. $U \perp_p V | Z$ if and only if $U \perp_{G^*} V | Z$.

Incremental associative Markov boundary algorithm (IAMB)

For each X_i do
  $Ad(X_i) := \varnothing$
  Repeat until no change occurs
    if there exists $X_j \notin Ad(X_i) \cup X_i$ such that $X_i \not\perp_p X_j | Ad(X_i)$ then
      $Ad(X_i) := Ad(X_i) \cup X_j$
  Repeat until no change occurs
    if there exists $X_j \in Ad(X_i)$ such that $X_i \perp_p X_j | Ad(X_i) \setminus X_j$ then
      $Ad(X_i) := Ad(X_i) \setminus X_j$

- **Exercise**. How would you perform score based structure learning for MNs ?

Contents

Thank you