732A96/TDDE15 Advanced Machine Learning

Graphical Models

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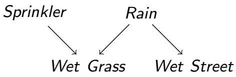
Lecture 3: Parameter Learning

Contents

Literature

- Main source
  - Bishop, C. M. *Pattern Recognition and Machine Learning*. Springer, 2006. Chapter 8.
- Additional source
  - Koski, T. J. T. and Noble, J. M. A Review of Bayesian Networks and Structure Learning. *Mathematica Applicanda* 40, 51-103, 2012.

Parameter Learning for BNs: Maximum Likelihood

DAG	Parameter values for the conditional probability distributions
	$q(s) = (0.3, 0.7) = (\theta_{s_0}, \theta_{s_1})$ $q(r) = (0.5, 0.5) = (\theta_{r_0}, \theta_{r_1})$ $q(wg \mid r_0, s_0) = (0.1, 0.9) = (\theta_{wg_0 \mid r_0, s_0}, \theta_{wg_1 \mid r_0, s_0})$ $q(wg \mid r_0, s_1) = (0.7, 0.3) = (\theta_{wg_0 \mid r_0, s_1}, \theta_{wg_1 \mid r_0, s_1})$ $q(wg \mid r_1, s_0) = (0.8, 0.2) = (\theta_{wg_0 \mid r_1, s_0}, \theta_{wg_1 \mid r_1, s_0})$ $q(wg \mid r_1, s_1) = (0.9, 0.1) = (\theta_{wg_0 \mid r_1, s_1}, \theta_{wg_1 \mid r_1, s_1})$ $q(ws \mid r_0) = (0.1, 0.9) = (\theta_{ws_0 \mid r_0}, \theta_{ws_1 \mid r_0})$ $q(ws \mid r_1) = (0.7, 0.3) = (\theta_{ws_0 \mid r_1}, \theta_{ws_1 \mid r_1})$ $p(s, r, wg, ws) = q(s)q(r)q(wg \mid s, r)q(ws \mid r)$

- In general,

$$q(X_i = k \mid Pa_i = j) = \theta_{X_i = k \mid Pa_i = j}$$

- Recall that

$$p(X_i = k \mid Pa_i = j) = q(X_i = k \mid Pa_i = j)$$

Parameter Learning for BNs: Maximum Likelihood

- Given a sample $d_{1:N}$, the log likelihood function is

$$\log p(d_{1:N}|\theta, G) = \log \prod_l p(d_l|\theta, G) = \log \prod_l \prod_i p(d_l[X_i]|d_l[Pa_i], \theta)$$

$$= \log \prod_l \prod_i \theta_{X_i=d_l[X_i]|Pa_i=d_l[Pa_i]} = \log \prod_i \prod_j \prod_k \theta_{X_i=k|Pa_i=j}^{N_{ijk}}$$

$$= \sum_i \sum_j \sum_k N_{ijk} \log \theta_{X_i=k|Pa_i=j}$$

  where N_{ijk} is the number of instances in $d_{1:N}$ with $X_i = k$ and $Pa_i = j$.

- To maximize the log likelihood function subject to the constraint $\sum_k \theta_{X_i=k|Pa_i=j} = 1$ for all i and j, we maximize

$$\sum_i \sum_j \sum_k N_{ijk} \log \theta_{X_i=k|Pa_i=j} + \sum_i \sum_j \lambda_{ij} (\sum_k \theta_{X_i=k|Pa_i=j} - 1)$$

  where λ_{ij} are called Lagrange multipliers.[1]

- Setting to zero the derivative with respect to $\theta_{X_i=k|Pa_i=j}$ gives

$$\theta_{X_i=k|Pa_i=j} = -N_{ijk}/\lambda_{ij}$$

- Replacing in the constraint gives $\lambda_{ij} = -N_{ij}$ and $\theta_{X_i=k|Pa_i=j}^{ML} = N_{ijk}/N_{ij}$.

[1] Any stationary point of the Lagrangian function is a stationary point of the original function subject to the constraints. Moreover, the log likelihood function is concave.

Parameter Learning for MNs: Iterative Proportional Fitting Procedure

- Given a complete sample $d_{1:N}$, the log likelihood function is

$$\log p(d_{1:N}|\theta, G) = \log \prod_l \frac{\prod_{K \in Cl(G)} \varphi(d_l[K])}{Z} = \sum_{K \in Cl(G)} \sum_k N_k \log \varphi(k) - N \log Z$$

  where N_k is the number of instances in $d_{1:N}$ with $K = k$. Then

$$\log p(d_{1:N}|\theta, G)/N = \sum_{K \in Cl(G)} \sum_k p_e(k) \log \varphi(k) - \log Z$$

  where $p_e(X)$ is the empirical probability distribution obtained from $d_{1:N}$.
- Let $Q \in Cl(G)$. The derivative with respect to $\varphi(q)$ is

$$\frac{\partial \log p(d_{1:N}|\theta, G)/N}{\partial \varphi(q)} = \frac{p_e(q)}{\varphi(q)} - \frac{1}{Z} \frac{\partial Z}{\partial \varphi(q)}$$

- Let $Y = X \setminus Q$. Then

$$\frac{\partial Z}{\partial \varphi(q)} = \sum_y \prod_{K \in Cl(G) \setminus Q} \varphi(k, \bar{k}) = \frac{Z}{\varphi(q)} \sum_y \prod_{K \in Cl(G) \setminus Q} \varphi(k, \bar{k}) \frac{\varphi(q)}{Z} = \frac{Z}{\varphi(q)} p(q|\theta, G)$$

  where $\bar{k}$ denotes the elements of q corresponding to the elements of $K \cap Q$.
- Putting together the results above, we have that

$$\frac{\partial \log p(d_{1:N}|\theta, G)/N}{\partial \varphi(q)} = \frac{p_e(q)}{\varphi(q)} - \frac{p(q|\theta, G)}{\varphi(q)}$$

Parameter Learning for MNs: Iterative Proportional Fitting Procedure

- Setting the derivative to zero gives [2]

$$\varphi^{ML}(q) = \varphi(q)p_e(q)/p(q|\theta, G)$$

No closed form solution but ...

IPFP

Initialize $\varphi(k)$ for all $K \in Cl(G)$
Repeat until convergence
    Set $\varphi(k) = \varphi(k)p_e(k)/p(k|\theta, G)$ for all $K \in Cl(G)$

- IPFP increases $\log p(d_{1:N}|\theta, G)$ in each iteration. So, it is globally optimal.
- Iterative coordinate ascend method.
- Note that computing $p(k|\theta, G)$ in the last line requires inference. Moreover, the multiplication and division are elementwise.
- Note also that Z needs to be computed in each iteration, which is computationally hard. This can be avoided by a careful initialization.

[2] The log likelihood function is concave.

Contents

- Parameter Learning for BNs
  - Maximum Likelihood
- Parameter Learning for MNs
  - Iterative Proportional Fitting Procedure

Thank you