Learning in Graphical Models

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Machine Learning

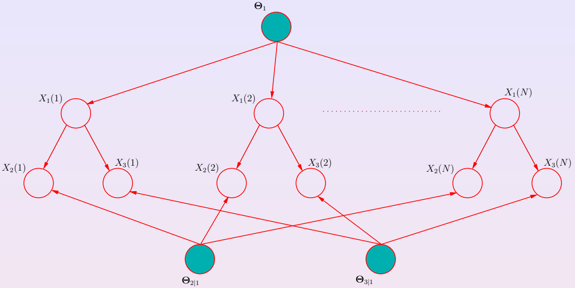
Learning graphical models

Parameter estimation

- We assume the structure of the model is given
- We are given a dataset of examples $\mathcal{D} = \{\mathbf{x}(1), \dots, \mathbf{x}(N)\}$
- Each example $\mathbf{x}(i)$ is a configuration for *all* (complete data) or *some* (incomplete data) variables in the model
- We need to estimate the parameters of the model (conditional probability distributions) from the data
- The simplest approach consists of learning the parameters maximizing the *likelihood* of the data:

$$\boldsymbol{\theta}^{\max} = \operatorname{argmax}_{\boldsymbol{\theta}} p(\mathcal{D}|\boldsymbol{\theta}) = \operatorname{argmax}_{\boldsymbol{\theta}} \mathcal{L}(\mathcal{D}, \boldsymbol{\theta})$$

Learning Bayesian Networks

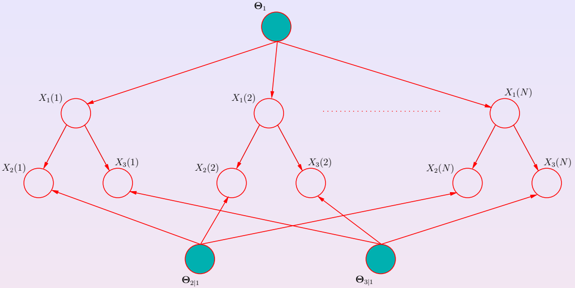


Maximum likelihood estimation, complete data

$$p(\mathcal{D}|\boldsymbol{\theta}) = \prod_{i=1}^{N} p(\mathbf{x}(i)|\boldsymbol{\theta}) \qquad \text{examples independent given } \boldsymbol{\theta}$$

$$= \prod_{i=1}^{N} \prod_{j=1}^{m} p(\mathbf{x}_j(i)|\mathrm{pa}_j(i), \boldsymbol{\theta}) \qquad \text{factorization for BN}$$

Learning Bayesian Networks



Maximum likelihood estimation, complete data

$$p(\mathcal{D}|\boldsymbol{\theta}) = \prod_{i=1}^{N}\prod_{j=1}^{m} p(\mathbf{x}_j(i)|\mathrm{pa}_j(i), \boldsymbol{\theta}) \qquad \text{factorization for BN}$$

$$= \prod_{i=1}^{N}\prod_{j=1}^{m} p(\mathbf{x}_j(i)|\mathrm{pa}_j(i), \boldsymbol{\theta}_{X_j|\mathrm{pa}_j}) \qquad \text{disjoint CPD parameters}$$

Learning graphical models

Maximum likelihood estimation, complete data

- The parameters of each CPD can be estimated independently:

$$\theta^{\max}_{X_j|\mathrm{Pa}_j} = \mathrm{argmax}_{\boldsymbol{\theta}_{X_j|\mathrm{Pa}_j}} \underbrace{\prod_{i=1}^{N} p(\mathbf{x}_j(i)|\mathrm{pa}_j(i), \boldsymbol{\theta}_{X_j|\mathrm{Pa}_j})}_{\mathcal{L}(\boldsymbol{\theta}_{X_j|\mathrm{Pa}_j},\mathcal{D})}$$

- A discrete CPD $P(X|\boldsymbol{U})$, can be represented as a table, with:
  - a number of rows equal to the number $Val(X)$ of configurations for X
  - a number of columns equal to the number $Val(\boldsymbol{U})$ of configurations for its parents $\boldsymbol{U}$
  - each table entry $\theta_{x|\mathbf{u}}$ indicating the probability of a specific configuration of $X = x$ and its parents $\boldsymbol{U} = \mathbf{u}$

Learning graphical models

Maximum likelihood estimation, complete data

- Replacing $p(x(i)|\mathrm{pa}(i))$ with $\theta_{x(i)|\mathbf{u}(i)}$, the local likelihood of a single CPD becames:

$$
\begin{aligned}
\mathcal{L}(\boldsymbol{\theta}_{X|\mathrm{Pa}}, \mathcal{D}) &= \prod_{i=1}^{N} p(x(i)|\mathrm{pa}(i), \boldsymbol{\theta}_{X|\mathrm{Pa}_j}) \\
&= \prod_{i=1}^{N} \theta_{x(i)|\mathbf{u}(i)} \\
&= \prod_{\mathbf{u} \in Val(\boldsymbol{U})} \left[\prod_{x \in Val(X)} \theta_{x|\mathbf{u}}^{N_{\mathbf{u},x}} \right]
\end{aligned}
$$

where $N_{\mathbf{u},x}$ is the number of times the specific configuration $X = x, \boldsymbol{U} = \mathbf{u}$ was found in the data

Learning graphical models

Maximum likelihood estimation, complete data

- A column in the CPD table contains a multinomial distribution over values of X for a certain configuration of the parents $\boldsymbol{U}$
- Thus each column should sum to one: $\sum_x \theta_{x|\mathbf{u}} = 1$
- Parameters of different columns can be estimated independently
- For each multinomial distribution, zeroing the gradient of the maximum likelihood and considering the normalization constraint, we obtain:

$$\theta_{x|\mathbf{u}}^{max} = \frac{N_{\mathbf{u},x}}{\sum_x N_{\mathbf{u},x}}$$

- The maximum likelihood parameters are simply the fraction of times in which the specific configuration was observed in the data

Learning graphical models

Adding priors

- ML estimation tends to overfit the training set
- Configuration not appearing in the training set will receive zero probability
- A common approach consists of combining ML with a prior probability on the parameters, achieving a maximum-a-posteriori estimate:

$$\boldsymbol{\theta}^{\max} = \text{argmax}_{\boldsymbol{\theta}} p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta})$$

Learning graphical models

Dirichlet priors

- The conjugate (read natural) prior for a multinomial distribution is a Dirichlet distribution with parameters $\alpha_{x|\mathbf{u}}$ for each possible value of x
- The resulting maximum-a-posteriori estimate is:

$$\theta_{x|\mathbf{u}}^{max} = \frac{N_{\mathbf{u},x} + \alpha_{x|\mathbf{u}}}{\sum_x \left(N_{\mathbf{u},x} + \alpha_{x|\mathbf{u}}\right)}$$

- The prior is like having observed $\alpha_{x|\mathbf{u}}$ imaginary samples with configuration $X = x, \boldsymbol{U} = \mathbf{u}$

Learning graphical models

Incomplete data

- With incomplete data, some of the examples miss evidence on some of the variables
- Counts of occurrences of different configurations cannot be computed if not all data are observed
- The full Bayesian approach of integrating over missing variables is often intractable in practice
- We need approximate methods to deal with the problem

Learning with missing data: Expectation-Maximization

E-M for Bayesian nets in a nutshell

- Sufficient statistics (counts) cannot be computed (missing data)
- Fill-in missing data inferring them using current parameters (solve inference problem to get *expected* counts)
- Compute parameters maximizing likelihood (or posterior) of such expected counts
- Iterate the procedure to improve quality of parameters

Learning with missing data: Expectation-Maximization

Expectation-Maximization algorithm

e-step Compute the expected sufficient statistics for the complete dataset, with expectation taken wrt the joint distribution for $\boldsymbol{X}$ conditioned of the current value of $\boldsymbol{\theta}$ and the known data $\mathcal{D}$:

$$\mathrm{E}_{p(\boldsymbol{X}|\mathcal{D},\boldsymbol{\theta})}[N_{ijk}] = \sum_{l=1}^{n} p(X_i(l) = x_k, \mathrm{Pa}_i(l) = \mathrm{pa}_j | \boldsymbol{X}_l, \boldsymbol{\theta})$$

- If $X_i(l)$ and $\mathrm{Pa}_i(l)$ are observed for $\boldsymbol{X}_l$, it is either zero or one
- Otherwise, run Bayesian inference to compute probabilities from observed variables

Learning with missing data: Expectation-Maximization

Expectation-Maximization algorithm

m-step compute parameters maximizing likelihood of the complete dataset D_c (using expected counts):

$$\boldsymbol{\theta}^* = \mathrm{argmax}_{\boldsymbol{\theta}} p(D_c|\boldsymbol{\theta})$$

which for each multinomial parameter evaluates to:

$$\theta^*_{ijk} = \frac{\mathrm{E}_{p(\boldsymbol{X}|\mathcal{D},\boldsymbol{\theta})}[N_{ijk}]}{\sum_{k=1}^{r_i} \mathrm{E}_{p(\boldsymbol{X}|\mathcal{D},\boldsymbol{\theta})}[N_{ijk}]}$$

Note

ML estimation can be replaced by maximum a-posteriori (MAP) estimation giving:

$$\theta^*_{ijk} = \frac{\alpha_{ijk} + \mathrm{E}_{p(\boldsymbol{X}|\mathcal{D},\boldsymbol{\theta},S)}[N_{ijk}]}{\sum_{k=1}^{r_i} \left(\alpha_{ijk} + \mathrm{E}_{p(\boldsymbol{X}|\mathcal{D},\boldsymbol{\theta},S)}[N_{ijk}]\right)}$$

Learning structure of graphical models

Approaches

constraint-based: test conditional independencies on the data and construct a model satisfying them

score-based: assign a score to each possible structure, define a search procedure looking for the structure maximizing the score

model-averaging: assign a prior probability to each structure, and average prediction over all possible structures weighted by their probabilities (full Bayesian, intractable)

Appendix: Learning the structure

Bayesian approach

- Let $\mathcal{S}$ be the space of possible structures (DAGS) for the domain $\boldsymbol{X}$.
- Let $\mathcal{D}$ be a dataset of observations
- Predictions for a new instance are computed marginalizing over both structures and parameters:

$$
\begin{aligned}
p(\boldsymbol{X}_{N+1}|\mathcal{D}) &= \sum_{S\in\mathcal{S}} \int_{\boldsymbol{\theta}} P(\boldsymbol{X}_{N+1}, S, \boldsymbol{\theta}|\mathcal{D}) d\boldsymbol{\theta} \\
&= \sum_{S\in\mathcal{S}} \int_{\boldsymbol{\theta}} P(\boldsymbol{X}_{N+1}|S, \boldsymbol{\theta}, \mathcal{D}) P(S, \boldsymbol{\theta}|\mathcal{D}) d\boldsymbol{\theta} \\
&= \sum_{S\in\mathcal{S}} \int_{\boldsymbol{\theta}} P(\boldsymbol{X}_{N+1}|S, \boldsymbol{\theta}) P(\boldsymbol{\theta}|S, \mathcal{D}) P(S|\mathcal{D}) d\boldsymbol{\theta} \\
&= \sum_{S\in\mathcal{S}} P(S|\mathcal{D}) \int_{\boldsymbol{\theta}} P(\boldsymbol{X}_{N+1}|S, \boldsymbol{\theta}) P(\boldsymbol{\theta}|S, \mathcal{D}) d\boldsymbol{\theta}
\end{aligned}
$$

Learning the structure

Problem

Averaging over all possible structures is too expensive

Model selection

- Choose a *best* structure S^* and assume $P(S^*|\mathcal{D}) = 1$
- Approaches:
  - Score-based:
    - Assign a score to each structure
    - Choose S^* to maximize the score
  - Constraint-based:
    - Test conditional independencies on data
    - Choose S^* that satifies these independencies

Score-based model selection

Structure scores

- Maximum-likelihood score:

$$S^* = argmax_{S \in \mathcal{S}} p(\mathcal{D}|S)$$

- Maximum-a-posteriori score:

$$S^* = argmax_{S \in \mathcal{S}} p(\mathcal{D}|S)p(S)$$

Computing $P(\mathcal{D}|S)$

Maximum likelihood approximation

- The easiest solution is to approximate $P(\mathcal{D}|S)$ with the maximum-likelihood score *over the parameters*:

$$P(\mathcal{D}|S) \approx max_{\theta} P(\mathcal{D}|S, \theta)$$

- Unfortunately, this boils down to adding a connection between two variables if their empirical mutual information over the training set is non-zero (proof omitted)
- Because of noise, empirical mutual information between any two variables is almost never exactly zero $\Rightarrow$ fully connected network

Computing $P(\mathcal{D}|S) \equiv P_S(\mathcal{D})$: Bayesian-Dirichlet scoring

Simple case: setting

- X is a single variable with r possible realizations (r-faced die)
- S is a single node
- Probability distribution is a multinomial with Dirichlet priors $\alpha_1, \ldots, \alpha_r$.
- $\mathcal{D}$ is a sequence of N realizations (die tosses)

Computing $P_S(\mathcal{D})$: Bayesian-Dirichlet scoring

Simple case: approach

- Sort $\mathcal{D}$ according to outcome:

$$\mathcal{D} = \{x^1, x^1, \ldots, x^1, x^2, \ldots, x^2, \ldots, x^r, \ldots, x^r\}$$

- Its probability can be decomposed as:

$$P_S(\mathcal{D}) = \prod_{t=1}^{N} P_S(X(t)|\underbrace{X(t-1), \ldots, X(1)}_{\mathcal{D}(t-1)})$$

- The prediction for a new event given the past is:

$$P_S(X(t+1) = x^k|\mathcal{D}(t)) = \mathrm{E}_{p_S(\boldsymbol{\theta}|\mathcal{D}(t))}[\theta_k] = \frac{\alpha_k + N_k(t)}{\alpha + t}$$

  where $N_k(t)$ is the number of times we have $X = x^k$ in the first t examples in $\mathcal{D}$

Computing $P_S(\mathcal{D})$: Bayesian-Dirichlet scoring

Simple case: approach

$$
\begin{aligned}
P_S(\mathcal{D}) &= \frac{\alpha_1}{\alpha}\frac{\alpha_1+1}{\alpha+1}\cdots\frac{\alpha_1+N_1-1}{\alpha+N_1-1} \\
&\cdot \frac{\alpha_2}{\alpha+N_1}\frac{\alpha_2+1}{\alpha+N_1+1}\cdots\frac{\alpha_2+N_2-1}{\alpha+N_1+N_2-1}\cdots \\
&\cdot \frac{\alpha_r}{\alpha+N_1+\cdots+N_{r-1}}\cdots\frac{\alpha_r+N_r-1}{\alpha+N-1} \\
&= \frac{\Gamma(\alpha)}{\Gamma(\alpha+N)}\prod_{k=1}^{r}\frac{\Gamma(\alpha_k+N_k)}{\Gamma(\alpha_k)}
\end{aligned}
$$

where we used the Gamma function ($\Gamma(x+1) = x\Gamma(x)$):

$$
\alpha(1+\alpha)\ldots(N-1+\alpha) = \frac{\Gamma(N+\alpha)}{\Gamma(\alpha)}
$$

Computing $P_S(\mathcal{D})$: Bayesian-Dirichlet scoring

General case

$$P_S(\mathcal{D}) = \prod_i \prod_j \frac{\Gamma(\alpha_{ij})}{\Gamma(\alpha_{ij} + N_{ij})} \prod_{k=1}^{r} \frac{\Gamma(\alpha_{ijk} + N_{ijk})}{\Gamma(\alpha_{ijk})}$$

where

- $i \in \{1, \ldots, n\}$ ranges over nodes in the network
- $j \in \{1, q_i\}$ ranges over configurations of X_i's parents
- $k \in \{1, r_i\}$ ranges over states of X_i

Note

The score is **decomposable**: it is the product of independent scores associated with the distribution of each node in the net

Search strategy

Approach

- Discrete search problem: NP-hard for nets whose nodes have at most $k > 1$ parents.
- Heuristic search strategies employed:
  - Search space: set of DAGs
  - Operators: add, remove, reverse one arc
  - Initial structure: e.g. random, fully disconnected, ...
  - Strategies: hill climbing, best first, simulated annealing

Note

Decomposable scores allow to recompute local scores only for a single move