Reliable and Efficient Inference of Bayesian Networks from Sparse Data by Statistical Learning Theory

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Summary. To learn (statistical) dependencies among random variables requires exponentially large sample size in the number of observed random variables if any arbitrary joint probability distribution can occur.

We consider the case that sparse data strongly suggest that the probabilities can be described by a simple Bayesian network, i.e., by a graph with small in-degree $\Delta$. Then this simple law will also explain further data with high confidence. This is shown by calculating bounds on the VC dimension of the set of those probability measures that correspond to simple graphs. This allows to select networks by structural risk minimization and gives reliability bounds on the error of the estimated joint measure without (in contrast to a previous paper) any prior assumptions on the set of possible joint measures.

The complexity for searching the optimal Bayesian networks of in-degree $\Delta$ increases only polynomially in the number of random variables for constant $\Delta$ and the optimal joint measure associated with a given graph can be found by convex optimization.

1. Bayesian networks and the causal Markov condition

Learning statistical dependencies among a set of $n$ random variables $X_1, \ldots, X_n$ is an important tool of scientific research. Formally, the task of learning those dependencies is to obtain some information about the joint probability measure $P$ where $P(x_1, \ldots, x_n)$ denotes the probability of the event $X_1 = x_1, \ldots, X_n = x_n$. A useful way to represent such information in a graphical way is given by the concept of Bayesian networks (Pearl, 1985).

Although one may consider Bayesian networks merely as a way of encoding statistical dependencies into a graph, the concept is better understood if a causal interpretation is given to the graph. Recall that every joint probability $P$ can be factorized as

$$P(x_1, x_2, \ldots, x_n) = \prod_{j=1}^{n} P(x_j | x_1, \ldots, x_{j-1}),$$

where $P(x_j | x_1, \ldots, x_{j-1})$ are the conditional probabilities given the values $x_1, \ldots, x_{j-1}$ of $X_1, X_2, \ldots, X_{j-1}$. Let $G$ be a directed acyclic graph. Assume that $G$ represents the underlying causal structure of $X_1, X_2, \ldots, X_n$. An arrow from $X_j$ to $X_i$ indicates that $X_j$ influences $X_i$ directly (here “directly” means that the causal effect is not intermediated by another variable $X_m$). Assume that the variables are ordered in a way that is consistent.

†Here we assume that each random variable $X_j$ can only take values in a finite set $\Omega_j$. 
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with $G$, i.e., there is no arrow from any $X_j$ to a variable $X_l$ with $l \leq j$. In case the variables $X_j$ correspond to definite and different times $t_j$, one may think of this order as the time order $t_1 < t_2 < \ldots < t_n$. Due to the fact that each $X_j$ is only (directly) influenced by its parents (the nodes with an arrow to $X_j$), we can give a simpler factorization for $P$ as follows:

$$P(x_1, x_2, \ldots, x_n) = \prod_j P(x_j|x_{j;1}, x_{j;2}, \ldots, x_{j;k_j}),$$

(1)

where $X_{j;1}, \ldots, X_{j;k_j}$ are the $k_j$ parents of $X_j$. It can be shown (Pearl, 2000) that this factorization implies the so-called Markov condition defined as follows.

**Definition 1.** Let $P$ be a joint probability distribution of $n$ random variables $X_1, X_2, \ldots, X_n$ and $G$ a directed acyclic graph with the variables as nodes. Then $P$ is said to satisfy the Markov condition relative to $G$ if for each variable $X_j$ the following condition holds:

- Given the values of all the parents of $X_j$, the variable $X_j$ is statistically independent from the set of those nodes $X_l$ with $l \neq j$ that are no (direct or indirect) descendants of $X_j$.

Here statistical independence of two sets $\mathcal{X} := \{X_1, \ldots, X_k\}, \mathcal{Y} := \{Y_1, \ldots, Y_l\}$ of variables given a third set $\mathcal{Z} := \{Z_1, \ldots, Z_m\}$ is defined by the condition

$$P(x_1, x_2, \ldots, x_k, y_1, y_2, \ldots, y_l|z_1, \ldots, z_m) = P(x_1, \ldots, x_k|z_1, \ldots, z_m)P(y_1, \ldots, y_l|z_1, \ldots, z_m)$$

for all possible assignments of the values $x_i, y_j, z_r$. Every graph $G$ defines a set of probability distributions.

**Definition 2.** Let $G$ be an arbitrary directed acyclic graph on $n$ nodes labeled with the random variables $X_1, \ldots, X_n$. Then $\mathcal{P}_G$ is the set of all joint probability distributions of $X_1, \ldots, X_n$ that satisfy the Markov condition relative to $G$.

Given an arbitrary order on $X_1, X_2, \ldots, X_n$ we define the complete acyclic graph $G_c$ corresponding to the order as the graph with an arrow from each $X_j$ to each $X_l$ with $l > j$. Note that every probability measure is Markovian relative to $G_c$. Hence one can find graphs $G$ such that $P$ is Markovian relative to $G$ by testing which edges can be removed from $G_c$ without violating the Markov property. Then a Bayesian network is formally defined as the pair $(G, P)$ where $G$ is a directed acyclic graph with random variables as nodes and $P$ a joint probability measure satisfying the Markov property relative to $G$.

Of course a graph $G$ does not necessarily coincide with the true causal structure when the measure is Markovian relative to $G$. We do not focus on the deep problem of inferring causal structure from statistics (Pearl, 2000). Here we mentioned the causal point of view only to emphasize that simple Bayesian networks may stem from a simple causal structure. The goal in this article is not to infer the causal structure but rather to infer properties of the probability measure from sparse data.

It is interesting to note that the graph $G$ determines directly the free parameters of those probability measures that are Markovian relative to $G$ since the probability measure $P$ is determined once the “transition probabilities” $P(x_j|x_{j;1}, x_{j;2}, \ldots, x_{j;k_j})$ are given. Once we have found a hypothetical graph with corresponding transition probabilities that seems to be in good agreement with the observed data we would like to judge whether we have really found a good model or whether the good agreement is rather caused by over-fitting our limited amount of data. In (Wocjan and Janzing, 2002) upper bounds on the required
sample size for learning the probabilities of all \( k \)-tuples \((x_{j_1}, x_{j_2}, \ldots, x_{j_k})\) with a certain accuracy and reliability are given. Under the assumption that the true probability measure is Markovian relative to a simple graph this will give the joint measure on the \( n \) variables up to a certain accuracy. Here we do not make any prior assumptions on the underlying joint probabilities. Merely the fact that we have found a simple model that does explain data shall give the accuracy and reliability of our guess.

For each node \( X_j \), the number of free parameters increases exponentially with the number \( k_j \) of parents of \( X_j \). Therefore it seems to be a reasonable concept to bound the number of free parameters of the available probability measures by considering graphs with small in-degree (i.e., the maximal number of parents) in order to avoid over-fitting. However, this is a heuristic argument. In the context of learning theory, Vapnik (1998) has argued that a small number of free parameters of the set of available functions to fit observed data is neither sufficient nor necessary to avoid over-fitting. He showed the so-called Vapnik-Chervonenkis (VC) dimension of a set of functions to be decisive. But we will show that it does make sense from the point of view of learning theory to consider graphs with small in-degree since we can derive upper bounds on the VC dimension of the set of corresponding probability measures.

In Section 2 we formulate the criterion for judging whether a hypothetical measure fits well the observed data and give a meaning on what defines a “good guess” of statistical dependencies, i.e. we define a risk functional quantifying the goodness of fit. In Section 3 we rephrase the concept of VC dimension and explain the general idea to use it for obtaining reliability bounds when an unknown function is to be learned. In our case the unknown function is the joint probability distribution on \( n \) random variables. Therefore we derive in Section 4 bounds on the VC dimension of sets of joint distributions corresponding to given graphs and sets of graphs. We show how to obtain reliability bounds for the estimated distribution. In Section 5 we show how to apply structural risk minimization principle in order to learn Bayesian networks reliably. In Section 6 we implement the minimization as a convex optimization problem.

### 2. Selection criterion for hypothetical networks

Assume the data are given by \( l \) \( n \)-tuples
\[
\mathbf{x}^1, \mathbf{x}^2, \ldots, \mathbf{x}^l.
\]

Using prior knowledge on the underlying causal structure we might prefer a specific graph \( G \). It should have the property that a probability distribution in \( \mathcal{P}_G \) describes the observed data already very well. In order to find the best distribution in \( \mathcal{P}_G \) we use the following approach (Vapnik, 1998). Consider the observed relative frequencies \( H(\mathbf{x}) \) formally as a probability measure over the set of possible \( n \)-tuples \( \Omega := \Omega_1 \times \Omega_2 \times \cdots \times \Omega_n \) and minimize the Kullback-Leibler relative entropy (Cover and Thomas, 1991)
\[
K(\hat{P} \mid H) := \sum_{\mathbf{x} \in \Omega} H(\mathbf{x}) \ln \hat{P}(\mathbf{x}) - \sum_{\mathbf{x} \in \Omega} H(\mathbf{x}) \ln H(\mathbf{x}),
\]
which is equivalent to the minimization of
\[
R_{emp}(\hat{P}) := \sum_{\mathbf{x}} H(\mathbf{x}) \ln \hat{P}(\mathbf{x}) = \frac{1}{l} \sum_{i \leq l} \ln \hat{P}(\mathbf{x}^i).
\]

(2)
over all $\tilde{P} \in \mathcal{P}_G$. By the law of large numbers $R_{\text{emp}}(\tilde{P})$ converges to

$$R(\tilde{P}) := \sum_{x \in \Omega} P(x) \ln \tilde{P}(x),$$

where $P$ is the true probability measure on $\Omega$. Note that $R(\tilde{P})$ yields for $\tilde{P} = P$

$$R(P) = \sum_{x \in \Omega} P(x) \ln P(x) = S(P),$$

i.e., the entropy of $P$. It measures the quality of the hypothesis concerning the statistical dependencies since it measures whether those events that have been predicted to be rather unlikely by the hypothetical measure do really occur rarely. Therefore a low value of $R(\tilde{P})$ does not only mean that the Kullback Leibler distance between $\tilde{P}$ and the true measure $P$ is low but it also implies that the entropy of $P$ is low. This means that we have found strong statistical dependencies. They may, for instance, indicate strong causal influences among the variables. This justifies to consider $R(\tilde{P})$ as a criterion that measures whether the hypothetical measure $\tilde{P}$ is not only good in the sense that its deviation from $P$ is small but also that we have found a law with high predictive power.

The minimization above is quite convenient since the factorization in eq. (1) corresponds to a sum of the logarithms of the conditional probabilities. It is clear that this minimization does not make sense if $G = G_c$ is the complete acyclic graph for a given order. Since all measures are in $\mathcal{P}_{G_c}$ we would clearly obtain $\tilde{P} = H$ – a fatal over-fit. This example shows intuitively that the minimization above leads to over-fitting when $G$ has too many arrows. In order to consider this problem from a perspective of statistical learning theory we rephrase the essential concepts in the next section.

3. Risk estimation by statistical learning theory

As explained above a major problem in inferring the true probability measure $P$ from the set of training data is over-fitting. It is not sufficient that $R_{\text{emp}}(\tilde{P})$ is small, we rather would like to have $R(\tilde{P})$ small. Abstractly speaking the problem reads: Given a family $(f_\alpha)$ of negative functions, consider the data points $x_1, x_2, \ldots, x_l$ and choose $f_\alpha$ in such a way that one can expect with high confidence that

$$R(f_\alpha) := -\sum_{x \in \Omega} f_\alpha(x)$$

is small. In this general setting the specific form of $f_\alpha$ is not relevant, the problem is simply to choose a function $f_\alpha$ from a family $(f_\alpha)$ such that its expectation value is maximal. Statistical learning theory tells the following. If the family $(f_\alpha)$ is small enough with respect to a specific measure we can say with high confidence that for all $\alpha$ the risk $R(f_\alpha)$ deviates from the empirical risk

$$R_{\text{emp}}(f_\alpha) := \frac{1}{l} \sum_{j \leq l} f_\alpha(x^j)$$

only by a small amount. (Note the slight abuse of notation. To be consistent, we should have written $R_{\text{emp}}(\ln \tilde{P})$ and $R(\ln \tilde{P})$ in Section 3 However, this should not lead to any confusions.) To make this precise we briefly explain the notion of VC dimension. First we introduce it only for two-valued functions (“indicator functions”, or “classifiers”).
Definition 3. Let $\Lambda$ be an index set of arbitrary cardinality. Let $(f_\alpha)_{\alpha \in \Lambda}$ be a set of indicator functions on $\Omega$. Then the $V_C$ dimension of $(f_\alpha)_{\alpha \in \Lambda}$ is the largest natural number $l$ such that there exists $l$ points $x_1, x_2, \ldots, x^l \in \Omega$ with the property that for every indicator function $\chi : \{x^1, x^2, \ldots, x^l\} \to \{0, 1\}$ there exists a function $f_\alpha$ such that its restriction to $\{x^1, x^2, \ldots, x^l\}$ coincides with $\chi$.

The definition of $V_C$ dimension of arbitrary real-valued functions relies on the $V_C$ dimension of sets of indicator functions:

Definition 4. Let $(f_\alpha)_{\alpha \in \Lambda}$ be a family of real-valued functions on a set $\Omega$. Then the $V_C$ dimension of $(f_\alpha)_{\alpha \in \Lambda}$ is the $V_C$ dimension of the family of the indicator functions ("classifiers") $(\chi_\mu \circ f_\alpha)_{\mu \in \mathbb{R}, \alpha \in \Lambda}$. Here $\chi_\mu$ is defined by $\chi_\mu(c) = 0$ for $c < \mu$ and $\chi_\mu(c) = 1$ for $c \geq \mu$.

The following theorem is a corollary from the statements in (Vapnik, 1998, pp.192, end of Section 5.3):

Theorem 5. Let $(f_\alpha)$ be a set of measurable real-valued functions on $\Omega$ bounded below and above by $A$ and $B$, respectively. Let $h$ be the $V_C$ dimension of the set. Then for any training data $x^1, x^2, \ldots, x^l$ we have with probability at least $1 - \eta$

$$R(f_\alpha) \leq R_{emp}(f_\alpha) + \phi_{A,B}(l, h, \eta)$$

with

$$\phi_{A,B}(l, h, \eta) := (B - A) \sqrt{\frac{h(\ln(2l/h) + 1) - \ln(\eta/4) + 1}{l}} \quad (5)$$

for all functions $f_\alpha$.

Note that the reliability bound is uniform on the family $(f_\alpha)$, i.e., with probability $1 - \eta$ the difference between $R_{emp}(f_\alpha)$ and $R(f_\alpha)$ is for all $f_\alpha$ bounded by the second term in eq. (5).

In the following section we will give bounds on the $V_C$ dimension of certain sets of joint probability distributions of $n$ variables.

4. The $V_C$ dimension associated with a graph or a set of graphs

The factorization of Markovian joint distributions in eq. (1) is decisive for the upper bound on the $V_C$-dimension of $\mathcal{P}_G$. Note that the $V_C$-dimension of the families

$$(\tilde{P})_{P \in \mathcal{P}_G}$$

and

$$(\ln \tilde{P})_{P \in \mathcal{P}_G}$$

coincide. Note furthermore that $\mathcal{P}_G$ contains also all distributions that are Markovian relative to a graph $G'$ whenever $G'$ was obtained from $G$ by deleting some arrows. In this sense, one considers always a set of graphs when general distributions in $\mathcal{P}_G$ are considered.

Let $m_j := |\Omega_j|$ the number of elements of $\Omega_j$. We find:
**Theorem 6.** Let $r_j$ be the indices of the set $P_j$ of parents of $X_j$ with respect to a given graph $G$. Then the VC-dimension of $P_G$ is at most

$$N_G := \sum_{j \leq n} \prod_{i \in (r_j \cup \{j\})} m_i .$$

**Proof.** We show that the logarithms of all probability distributions in $P_G$ can be written as a linear functional in a common $N_G$ dimensional vector space. For each set $j = \{j_1, \ldots, j_k\} \subset \{1, \ldots, n\}$ we define

$$\Omega_j := \Omega_{j_1} \times \Omega_{j_2} \times \ldots \times \Omega_{j_k} .$$

Then we define the vector space $V_j$ as the set of real-valued functions on $\Omega_{r_j \cup \{j\}}$.

The dimension of $V_j$ is clearly given as

$$\prod_{i \in (r_j \cup \{j\})} m_i .$$

By setting

$$V := \oplus_{j \leq n} V_j$$

we obtain a vector space of dimension $N_G$. Now we define a vector $f_j \in V_j$ by

$$f_j(x_j, p_j) := \ln P(x_j | p_j)$$

and

$$f := \oplus_{j \leq n} f_j .$$

For each $n$-tuple $x := (x_1, \ldots, x_n)$ we define a vector

$$e^x := \oplus_j e^x_j \in V$$

where each vector $e^x_j$ is 1 for the entry that corresponds to the restriction of $x$ to $p_j \cup \{j\}$ and 0 for all the other values. Then the logarithm of the probability of $x$ can be obtained by

$$\ln P(x_1, \ldots, x_n) = \langle e^x | f \rangle .$$

This shows that the logarithm can be written as linear functional in $V$. The VC dimension of the set of linear functions in $\mathbb{R}^N$ is $N$ (Vapnik, 1998). This completes the proof.

The idea of the proof is quite similar to the proof of Lemma 2 in (Herrmann and Janzing, 2003). There we have given an upper bound on the VC dimension of the set of so-called $k$-factor log-linear models. These are probability distributions with the property that their logarithm can be written as a sum of functions depending on $k$ variables only. Here we have considered a specific factorization corresponding to a given graph. This prior knowledge decreases the VC-dimension.

Now we consider the case that no specific graph is given but all graphs with a given in-degree are allowed which respect a given order on the set of random variables. We find:
Theorem 7. Let $X_1 < X_2 < \ldots < X_n$ be an ordering on the set of random random variables. Let $\mathcal{P}_\Delta$ be the set of all measures that are Markovian relative to an appropriate graph with in-degree $\Delta$ which is consistent with the order, i.e., there are only arrows from $X_i$ to $X_j$ for $i < j$. Then the VC dimension of $\mathcal{P}_\Delta$ is at most

$$N_\Delta := \sum_{j=1}^{n} \prod_{i \in j} m_i m_{i_1} \ldots m_{i_\Delta},$$

where the second sum runs over all $\Delta$-subsets $i := \{i_1, i_2, \ldots, i_\Delta\}$ of $\{1, \ldots, j-1\}$.

Proof. We extend the proof of Theorem 6. The definition of each space $V_j$ given there depends on one particular choice of the parents of $X_j$. Now we have a vector space $\hat{V}_i$ corresponding to each possible choice of parents of $X_j$ given by one specific $\Delta$-subset $i$ for each node $j$. We define

$$\hat{V} := \bigoplus_{j \leq n} \bigoplus_{i} V^i_j.$$

One checks easily that $N_\Delta$ is the dimension of $\hat{V}$. Note furthermore that also the definition of each $c^x_j$ in the proof of Theorem 6 depends on one specific choice $i$ of the parents of $X_j$. Hence we obtain now a different vector $c^x_j$ for each $i$. In analogy to the proof of Theorem 6 we assign a vector $\hat{c}^x$ to each $n$-tuple $x = (x_1, \ldots, x_n)$ by

$$\hat{c}^x := \bigoplus_{j} \bigoplus_{i} c^x_{ji}.$$

Let $\tilde{P}$ be an arbitrary probability measure in $\mathcal{P}_\Delta$. The proof of Theorem 6 assigns a vector $f \in V$ to this measure. Note that there is a canonical embedding of the vector space $V$ introduced in the proof of Theorem 6 into the space $\hat{V}$ defined here since each $V_j$ defined there corresponds to one specific $V^i_j$ here. With this embedding we have

$$\ln \tilde{P}(x_1, \ldots, x_n) = \langle \hat{c}^x | f \rangle.$$

Hence the logarithms of probabilities can be written as an inner product in a vector space of dimension $N_\Delta$. This completes the proof.

If no specific order on the random variables is given a priori the VC dimension of all graphs with a fixed in-degree is bounded as follows:

Theorem 8. Let $\mathcal{P}_\Delta$ be the set of probability measures that are Markovian relative to some graph $G$ with in-degree $\Delta$. Then the VC dimension of $\mathcal{P}_\Delta$ is at most

$$N_\Delta := \sum_j \prod_{i \in j} m_i,$$

where the sum runs over all $(\Delta + 1)$-subsets $j$ of $\{1, 2, \ldots, n\}$.

The proof follows from the observation that each $P \in \mathcal{P}_\Delta$ is a $(\Delta + 1)$-factor log-linear model, i.e., a probability distribution with the property that its logarithm can be written as a sum of functions each depending on at most $\Delta + 1$ variables. Then the bound of Lemma 2 in (Herrmann and Janzing, 2003) applies.

The following corollary from Theorem 6 shows explicitly how to use the bounds on the VC-dimensions in order to get reliability bounds on the estimated risk functional. Note that
it is therefore necessary to restrict one’s attention to sets of probability measures which are bounded below. Explicitly, we define: Let \( \mathcal{P}^\lambda \) for each \( \lambda > 0 \) be the set of joint distributions \( \tilde{P} \) with the property that
\[
\tilde{P}(x_1, x_2, \ldots, x_n) \geq \lambda
\]
for all \( n \)-tuples in \( \Omega \). Note that we do not assume that the true probability measure \( P \) satisfies this requirement. Only the hypothetical measure \( \tilde{P} \) has to be bounded. Then the bounds \( A \) and \( B \) in Theorem 5 are 0 and \( -\ln \lambda \), respectively. We conclude:

**Corollary 1.** Let \( \mathcal{P} \subset \mathcal{P}^\lambda \) be a set of joint distributions with VC-dimension \( h \). Then for any training data \( x^1, x^2, \ldots, x^l \) we have with probability at least \( 1 - \eta \)
\[
R(\tilde{P}) \leq R_{emp}(\tilde{P}) + \phi_\lambda(l, h, \eta)
\]
with
\[
\phi_\lambda(l, h, \eta) := (-\ln \lambda) \sqrt{\frac{h(\ln(2l/h) + 1) - \ln(\eta/4) + 1}{l}}
\]
(8)
uniformly for all \( \tilde{P} \in \mathcal{P} \).

Setting \( \mathcal{P} := \mathcal{P}_G^\lambda \) we obtain reliability bounds on the estimated probability measure provided that the graph \( G \) has been chosen in advance. With \( \mathcal{P} := \mathcal{P}_G^\lambda \) we obtain reliability bounds if the hypothetical measures are restricted to those that factorize to a “simple” graph (in the sense of small in-degree).

However, the prior restriction to a specific \( \lambda \) and a specific graph or to graphs with small in-degree is not acceptable. An appropriate way to learn Bayesian networks should also consider complex graphs provided that sufficiently large sampling strongly indicate a more complicated dependency among the variables. Similarly, one should not a priori exclude probabilities that are smaller than a specific value \( \lambda \). For large sample size data may give strong evidence that some probabilities are indeed small. On the other hand, the estimation in Corollary 1 seems to require prior restrictions.

This problem is solved by structural risk minimization principle (Vapnik, 1995 and 1998) in statistical learning theory. It uses a hierarchy of increasing sets of hypothetical functions. Then a function \( g \) from a larger set is only preferred compared to a function \( f \) from a smaller set if not only \( R_{emp}(g) < R_{emp}(f) \) but also the bound on \( R(g) \) is smaller than the bound on \( R(f) \). We explain this principle in the following section.

Now we briefly summarize the estimations for the VC dimension of some interesting set of graphs. Here we assume that \( l \) is the maximum over all values \( m_j \).

- For the VC dimension of a given graph \( G \) with in-degree \( \Delta \) we have
  \[
h \leq nl^{\Delta+1}.
\]
This follows from Theorem 6 since
\[
\prod_{i \in \{r \cup \{j\} \}} m_i \leq l^{\Delta+1}.
\]

- For the VC dimension of all graphs with in-degree \( \Delta \) which respect a given order on the nodes we have
  \[
h \leq l^{\Delta+1} \sum_{j=1}^{n} \binom{j-1}{\Delta}.
\]
This is due to Theorem 7 since the second sum in eq. \(7\) runs over 
\[
\binom{j-1}{\Delta}
\]
terms.

- For the VC dimension of the set of all graphs with in-degree \(\Delta\) we have 
\[
h \leq \binom{n}{\Delta + 1} l^{\Delta + 1}.
\]
This follows from Theorem 8 since the sum in eq. \(7\) runs over 
\[
\binom{n}{\Delta + 1}
\]
terms.

This seems to suggest that in general a small in-degree reduces the VC dimension considerably whereas prior knowledge on the causal order is less relevant.

5. Structural risk minimization

Before we apply structural risk minimization to the problem of learning probabilities we briefly sketch the general idea. Consider the case that an arbitrary function on a set \(\Omega\) is to be learned. Define a sequence \((F_k)_{k \in \mathbb{N}}\) of families \(F_k\) of functions. The idea is that the sequence defines a hierarchy of more and more complex families of functions and the less complex ones are a priori preferred. Let \((p_k)_{k \in \mathbb{N}}\) be any sequence of non-negative numbers with \(\sum_k p_k = 1\). These values express to what extent one tends to prefer functions from \(F_k\) with lower \(k\). Let \(h_k\) be the VC-dimension of \(F_k\). Then one has with probability \(1 - \eta\) that for each function \(f \in \bigcup_k F_k\)
\[
R(f) \leq R_{emp}(f) + \phi(h_k, l, p_k \eta),
\]
where \(\phi\) is the confidence term in eq. \(5\). This is a standard union bound argument (see e.g. Herbrich, 2002). Note that the sequence on \(p_k\) may be chosen in such way that it expresses prior probabilities to the choice of a certain class \(F_k\). But it should be emphasized that the reliability bound in eq. \(9\) does not rely on this interpretation.

Here we define a hierarchy of probability measures which takes into account two aspects of a measure: We prefer measures which are Markovian relative to a simple graph and measures with high cut-off value \(\lambda\). Let \((\lambda_m)_{m \in \mathbb{N}}\) be a sequence of positive values converging to zero. Let \(\mathcal{P}^{\lambda_m}\) be the set of probability measures bounded from below by \(\lambda_m\). Let \(\mathcal{P}_1, \ldots, \mathcal{P}_r\) be \(r\) sets of probability measures. They may, for instance, correspond to an enumeration of all directed acyclic graphs on \(n\) nodes. They may also correspond to graphs with in-degree \(1, 2, \ldots, r\). Then we prefer probability measures in \(\mathcal{P}_k \cap \mathcal{P}^{\lambda_m}\) for small \(m\) and small \(k\). We may express this by defining probabilities \(q_{k,m}\) which are decreasing in \(k\) and \(m\). In analogy to the bound above we obtain:
Theorem 9. Let \(( \mathcal{P}_k )_{k \in K} \) with \( K = \mathbb{N} \) or \( K = \{1, \ldots, r\} \) an arbitrary set of families of joint distributions on the \( n \) random variables.
Let \(( q_{k,m} )_{k,m} \) define an arbitrary probability measure on \( K \times \mathbb{N} \). Let \( h_k \) be the VC-dimension of \( \mathcal{P}_k \). Then we know with probability \( 1 - \eta \) for all \( k \leq r, m \in \mathbb{N} \) and all \( \tilde{P} \in \mathcal{P}_k \cap \mathcal{P}^\lambda_m \)

\[
R(\tilde{P}) \leq R_{\text{emp}}(\tilde{P}) + \phi_\lambda(h_k, l, q_{k,m}\eta)
\]

holds, with

\[
\phi_\lambda(h_k, l, q_{k,m}\eta) := - \ln \lambda_m \sqrt{\frac{h_k(\ln(2l/h_k) + 1) - \ln(q_{k,m}\eta/4) + 1}{l}}
\]

The structural risk minimization principle works as follows. For a given number \( k, m \) choose \( \tilde{P}_{k,m} \in \mathcal{P}^\lambda_m \cap \mathcal{P}_k \) such that \( R_{\text{emp}}(\tilde{P}_{k,m}) \) is minimal. Then choose \( k, m \) such that

\[
R_{\text{emp}}(\tilde{P}_{k,\lambda}) + \phi_\lambda(l, h, q_{k,m}\eta)
\]

is minimal.

The following example gives an idea how to apply this principle. Given \( n \) binary variables. Then our upper bound on the VC dimension of the set of graphs with in-degree \( \Delta \) is

\[
h_\Delta \leq n 2^{\Delta+1}.
\]

Let \( \mathcal{P}_k \) be the set of joint distributions which are Markovian relative to a graph with in-degree \( k \). Set furthermore \( \lambda_m = 2^{-m} \) and choose the prior probability measure on \( \mathbb{N} \times \mathbb{N} \) as

\[
q_{k,m} := 2^{-k-m}.
\]

For \( \tilde{P} \in \mathcal{P}_k \cap \mathcal{P}^\lambda_m \) we obtain

\[
\phi_\lambda(l, h, q_{k,m}\eta) = m \ln 2 \sqrt{n2^{k+1}(\ln(2l/(n2^{k+1})) + 1) - \ln(q_{k,m}\eta/4) + (k + m) \ln 2 + 1}
\]

The confidence term grows exponentially in \( k \), with \( O(\sqrt{n}) \) and with \( O(m^{3/2}) \) whenever the other parameters are fixed. Hence the required sample size grows quickly with the in-degree, whereas the number of random variables is less decisive. Also the cut-off value \( \lambda \) of the probabilities is less decisive since the required sample size grows only with \( O(m^{3/2}) \) although we have defined the cut-off values \( \lambda_m \) in such a way that they decrease exponentially in \( m \).

6. Convex Optimization for Bayesian networks

The number of directed acyclic graphs with constant in-degree \( \Delta \) and \( n \) nodes increases polynomially in \( n \). Therefore it is realistic to assume that for all graphs with small in-degree ("sparse graphs") the optimization can be carried out for each graph. Hence we may restrict our attention to finding the optimal probability measure that is Markovian relative to a given graph \( G \) and bounded by a given value \( \lambda \) from below. Let \( V_j \) be defined as in the proof of Theorem 6, i.e., the set of real-valued functions on

\[
\Omega_{r_j \cup \{j\}}.
\]
Let $\mathbf{x}^i$ be the $i$-th observed $n$-tuple. Let $\mathbf{x}^i|_{r_j \cup \{j\}}$ its restriction to the variable $X_j$ and all its parents. Then the task is to find a vector

$$f = \oplus f_j \in \oplus V_j = V$$

that minimizes

$$R_{\text{emp}}(f) := \frac{1}{l} \sum_{i \leq l} \sum_{j \leq n} f_j(\mathbf{x}^i|_{r_j \cup \{j\}})$$

subject to the following constraints:

(a) For each $j$ the sum of the conditional probabilities $P(x_j|\omega)$ over all $x_j \in \Omega_j$ has to be 1 for all $\Delta$-tuples $\omega \in \Omega_{p_j}$. Formally this means

$$Z_{\omega}(f_j) := \exp(\sum_{x_j \in \Omega_j} f_j(x_j, \omega)) = 1$$

for $\omega \in \Omega_{p_j}$.

(b) No probability $P(x_1, \ldots, x_n)$ is less than $\lambda$. We can achieve this by stating the stronger constraint that no transition probability $P(x_j|\omega)$ is less than $\lambda^{1/n}$. This is equivalent to

$$G_{\omega,j,x_j}(f) := f_j(x_j, \omega) \geq \frac{1}{n} \ln \lambda.$$ 

The optimization is rather similar to that one in (Herrmann and Janzing, 2003) with the decisive difference that the normalization can be performed for each node separately here whereas the normalization condition for the joint measure on $n$ variables involves a sum over all possible $n$-tuples, i.e., a number growing exponentially in $n$. Here the computational complexity grows only polynomially in $n$ for constant $k$. The number of constraints grows linearly in $n$ but exponentially in $k$. The number of terms in the sum (11) grows also exponentially in $k$. But since we assume that $k$ is small we consider the optimization as computationally tractable. Due to the convexity of the constraints (see Herrmann and Janzing, 2003) it is a usual linear programming problem that can be efficiently solved (Pallaschke and Rolewicz, 1997).

### 7. Conclusions

We have presented a method for estimating the joint distribution of a large number of random variables from sparse data. The statistical dependencies among the variables are explained by Bayesian networks such that networks with simple graphs are preferred. We provide reliability bounds without restricting the set of joint distribution under consideration. We have shown that the set of probability measures that are markovian relative to simple graphs have low VC-dimension. This guarantees reliable estimation in the sense of statistical learning theory whenever the observed data is explained well by those “simple measures”. If no simple Bayesian network fits the data the method does not allow reliable estimation. Furthermore we have shown that finding the optimal distribution within a class of distributions (markovian relative to a given graph) is a convex optimization problem. Since the number of simple graphs is not too large, the whole estimation can be performed efficiently.
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