

# Required sample size for learning sparse Bayesian networks with many variables

Paweł Wocjan\*, Dominik Janzing, and Thomas Beth

Institut für Algorithmen und Kognitive Systeme, Universität Karlsruhe,  
Am Fasanengarten 5, D-76 131 Karlsruhe, Germany

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## Abstract

Learning joint probability distributions on  $n$  random variables requires exponential sample size in the generic case. Here we consider the case that a temporal (or causal) order of the variables is known and that the (unknown) graph of causal dependencies has bounded in-degree  $\Delta$ . Then the joint measure is uniquely determined by the probabilities of all  $(2\Delta + 1)$ -tuples. Upper bounds on the sample size required for estimating their probabilities can be given in terms of the VC-dimension of the set of corresponding cylinder sets. The sample size grows less than linearly with  $n$ .

## 1 Introduction

Learning joint probability measures on a large set of variables is an important task of statistics. One of the main motivations to estimate joint probabilities is to study statistical dependencies and independencies between the random variables [6]. In many applications the goal is to obtain information on the underlying causal structure that produces the statistical correlations. However, the problem of learning causal structure from statistical data is in general a deep problem and cannot be solved by statistical considerations alone [6, 3].

Here we do not focus on the problem of uncovering the causal structure, we rather address the problem of learning the probability distribution on a large set of variables. In general, the sample size required for estimating an unknown measure on the variables  $X_1, \dots, X_n$  grows exponentially with  $n$ . Assume for simplicity that each  $X_j$  is a discrete

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\*e-mail: {wocjan,janzing,eiss\_office}@ira.uka.de

variable with  $d$  possible values. Then the probabilities of  $d^n$  possible outcomes have to be estimated. The sample size can be decreased considerably if prior knowledge on the possible correlations is given. Consider for example the trivial case when no statistical dependencies are possible at all, i.e.,

$$P(x_1, x_2, \dots, x_n) = P(x_1)P(x_2) \dots P(x_n),$$

where  $x_j$  denotes particular realizations of the corresponding variable  $X_j$ . Then one has only to learn the probabilities  $P(x_1), \dots, P(x_n)$ .

There are less trivial examples where prior information on the statistical dependencies strongly reduce the required sample size. For instance, this information may stem from knowledge on the underlying causal structure. Following [6, 7] we encode causal structure in a directed graph with random variables as its nodes. Here we assume the graph to be acyclic. The decisive prior information assumed to be given here is that each variable has at most  $\Delta$  parents, i.e., is influenced directly by at most  $\Delta$  other nodes. Note that we do not assume that we know which nodes are the parents. Therefore, our assumption is merely a kind of *simplicity assumption* on the causation for the statistical dependencies. Furthermore, it should be emphasized that in many cases one will not find any pair of variables that are statistically independent. The constraints on the causal structure for the joint probability measure are more sophisticated and are only reflected in *conditional* probabilities. These constraints are well-known as the *Markov condition* in *Bayesian networks* [6, 3]. Conversely, Bayesian networks may be considered as a convenient and intuitive way of encoding statistical dependencies among variables in a graph (without any causal interpretation).

## 2 Bayesian networks

Let us briefly introduce Bayesian networks. To do that we define *conditional independence* relationships among variables, a central notion in the analysis of probability distributions.

### Definition 1 (Conditional independence)

Let  $\mathbf{V} = \{X_1, X_2, \dots, X_n\}$  be a finite set of variables. Let  $P(\cdot)$  be a joint probability distribution over the variables in  $V$ , and let  $\mathbf{X}$ ,  $\mathbf{Y}$  and  $\mathbf{Z}$  stand for any three subsets of  $\mathbf{V}$ . The sets  $\mathbf{X}$  and  $\mathbf{Y}$  are said to be conditionally independent given  $\mathbf{Z}$ , denoted by

$$(\mathbf{X} \perp \mathbf{Y} \mid \mathbf{Z}) \tag{1}$$

if

$$P(\mathbf{x}, \mathbf{y} \mid \mathbf{z}) = P(\mathbf{x} \mid \mathbf{z})P(\mathbf{y} \mid \mathbf{z}), \quad \text{whenever } P(\mathbf{z}) > 0, \tag{2}$$

where  $\mathbf{x}$  is the tuple denoting a particular realization of the values of the variables in  $\mathbf{X}$  and the tuples  $\mathbf{y}$  and  $\mathbf{z}$  are defined analogously. In words, if all the actual values of the variables in  $\mathbf{Z}$  are known the actual values of the variables in  $\mathbf{Y}$  do not provide any further information on the actual values of the variables in  $\mathbf{X}$ .

Directed acyclic graphs or Bayesian networks – a term coined in [4] – are used to facilitate economical representation of joint probability distributions. The basis decomposition scheme offered by directed acyclic graphs can be illustrated as follows. Let  $P(\cdot)$  be a joint probability distribution as in Definition 1. The chain rule of probability calculus always permit to decompose  $P$  as a product of  $n$  conditional probability distributions:

$$P(x_1, \dots, x_n) = \prod_{j=1}^n P(x_j | x_1, \dots, x_{j-1}). \quad (3)$$

Now suppose that the conditional probability of some variable  $X_j$  is not sensitive to all the predecessors of  $X_j$  but only to a small subset of those predecessors. In words, suppose that  $X_j$  is independent of all other predecessors, once we know the values of a selected group of predecessors called  $\mathbf{P}_j := \{X_{j,1}, \dots, X_{j,m_j}\}$ . We can then write

$$P(x_1, \dots, x_n) = \prod_{j=1}^n P(x_j | \mathbf{p}_j) \quad (4)$$

considerably simplifying the input information. Instead of specifying the probability of  $X_j$  conditional on all possible realizations of its predecessors  $X_1, \dots, X_{j-1}$ , we need only to take into account the possible realizations of the set  $\mathbf{P}_j$ . The set  $\mathbf{P}_j$  is called the *Markovian parents* of  $X_j$ , or the *parents* for short. The reason for the name becomes clear when we introduce graphs around this concept.

**Definition 2 (Markov parents)**

Let  $V = \{X_1, \dots, X_n\}$  be an ordered set of variables, and let  $P(\cdot)$  be the joint probability distribution on these variables. A set of variables  $\mathbf{P}_j$  is said to be Markovian parents of  $X_j$  if  $\mathbf{P}_j$  is a minimal set of predecessors of  $X_j$  that renders  $X_j$  independent of all its other predecessors. In words,  $\mathbf{P}_j$  is any subset of  $\{X_1, \dots, X_{j-1}\}$  satisfying

$$P(x_j | \mathbf{p}_j) = P(x_j | x_1, \dots, x_{j-1}) \quad (5)$$

such that no proper subset of  $\mathbf{P}_j$  satisfies Eq. (5).

This definition assigns to each variable  $X_j$  a selected set  $\mathbf{P}_j$  of preceding variables that are sufficient for determining the probability of  $X_j$ . The values of the other preceding variables are redundant once we know the values  $\mathbf{p}_j$  of the parent set  $\mathbf{P}_j$ . This assignment can be encoded in a directed acyclic graph in which the variables are

represented by the nodes and arrows are drawn from each node of the parent set toward the child node  $X_j$ .

Furthermore, Definition 2 also provides a simple recursive method for constructing such a DAG: Starting with the pair  $(X_1, X_2)$ , we draw an arrow from  $X_1$  to  $X_2$  if and only if the two variables are dependent. Assume that we have constructed the DAG up to node  $j - 1$ . At the  $j$ th stage, we select any minimal set of predecessors of  $X_j$  that renders  $X_j$  independent from its other predecessors (as in Eq. (5)), call this set  $\mathbf{P}_j$  and draw an arrow from each member in  $\mathbf{P}_j$  to  $X_j$ . The result is a directed acyclic graph, called a Bayesian network, in which an arrow from  $X_i$  to  $X_j$  assigns  $X_i$  as a Markovian parent of  $X_j$ , consistent with Definition 2.

Let us mention that the set  $\mathbf{P}_j$  is unique whenever the distribution  $P(\cdot)$  is strictly positive, i.e. every configuration of variables, no matter how unlikely, has some finite probability of occurring. Under such conditions, the Bayesian network associated with  $P(\cdot)$  is unique, given the ordering of the variables [5].

### Definition 3 (Markov Compatibility)

Let  $G$  be a DAG. If a probability distribution  $P$  admits a factorization relative to  $G$ , i.e.

$$P(x_1, \dots, x_n) = \prod_{j=1}^n P(X_j = x_j | \mathbf{P}_j = \mathbf{p}_j), \quad (6)$$

where  $\mathbf{P}_j$  are the parents of the node  $X_j$  defined by the graph  $G$ , then we say  $G$  and  $P$  are compatible, or that  $P$  is Markov relative to  $G$ .

The problem of learning a Bayesian network usually treated in the literature is as follows. Given a *training set*  $\{\mathbf{x}^1, \dots, \mathbf{x}^l\}$ , find a network that *best matches* the training set (see e.g. [1, 2]), i.e. to determine a graph  $G$  such that  $P$  is Markov relative to  $G$ .

## 3 Networks with bounded in-degree

To motivate our decisive assumption we would like to note that scientific reasoning always tries to find a simple explanation for the data (“Occam’s Razor”). We are aware of the fact that “simplicity” is hard to formalize. However, it seems reasonable to try to explain data by *simple causal graphs*. Here we may use the *in-degree* of the graph as criterion for simplicity. It is defined as the greatest number of parents that occurs. The intuitive meaning of in-degree  $\Delta$  is that no variable is directly influenced by more than  $\Delta$  others. For  $\Delta \ll n$  we call the graph *sparse*. Clearly, the in-degree is only one of the graph theoretical notions that may be used to define *simplicity* of causal explanations; we could use e.g. the number of edges.

Let  $G$  be an arbitrary DAG with in-degree  $\Delta$ . Then every probability measure that is Markovian relative to  $G$  is already determined by the probabilities of all  $(\Delta + 1)$ -tuples. This follows directly from the decomposition in Eq. (5) since the conditional probabilities  $P(x_j | \mathbf{p}_j)$  are the quotients of the probabilities  $P(x_j, \mathbf{p}_j)$  and  $P(\mathbf{p}_j)$  of sizes at most  $\Delta + 1$  and  $\Delta$ , respectively. Consequently, if  $G$  is known we can learn the probability measure  $P$  by learning the probabilities of all  $\Delta + 1$ -tuples.

In contrast, we do not assume that we know the exact structure of  $G$  but only that its in-degree is at most  $\Delta$ . Now the situation is more complicated. Since we do not know the set of parents for any  $X_j$ , we do not know which conditional probabilities have to appear in the factorization in Eq. (5). Therefore, it is not sufficient to know the probabilities of all tuples of size  $\Delta + 1$  to reconstruct the structure. We have to know the probabilities of at least all  $(\Delta + 2)$ -tuples to be able to *test* conditional independencies. The following theorem shows that it is *sufficient* to know the probabilities of all  $(2\Delta + 1)$ -tuples.

**Theorem 4 (Graph structure from correlations)**

*Let  $X_1 < X_2 < \dots < X_n$  be an ordering of the variables. Assume that  $P$  is a probability measure that is Markov relative to a directed acyclic graph (DAG)  $G$ . Let  $G$  be consistent with the ordering, i.e., the graph  $G$  contains no arrow from  $X_j$  to  $X_i$  for  $i < j$ . Let  $G$  have in-degree  $\Delta$  and assume that the probabilities of all  $(2\Delta + 1)$ -tuples are known. Then we can find a graph  $\tilde{G}$  (possibly different from  $G$ ) that is Markov relative to  $P$  and has at most in-degree  $\Delta$ .*

**Proof:** We can find the correct graph structure by the following iteration: Draw an arrow from  $X_1$  to  $X_2$  if the two variables are dependent. Assume we have found the correct structure on  $X_1, X_2, \dots, X_{j-1}$ .

In order to find a possible minimal set  $\mathbf{P}_j$  of parents of  $X_j$  we proceed as follows: Let  $m := \min\{j - 1, \Delta\}$ . For each  $m$ -subset  $K \subseteq V_j := \{X_1, X_2, \dots, X_{j-1}\}$  test whether the following statement is true:

$(X_j \perp L | K)$  for all sets  $L$  (disjoint from  $K$ ) that contain at most  $m$  elements.

If this is true,  $K$  contains necessarily a set  $\mathbf{P}'_j$  that can be taken as Markovian parents of  $X_j$ . This can be seen as follows: Choose  $L$  such that  $(L \cup K) \supseteq \mathbf{P}_j$  for an arbitrary minimal choice of parents of  $X_j$ . This is possible since  $X_j$  has at most  $m$  parents. Since  $L \cup K$  contains the parents of  $X_j$  it renders  $X_j$  independent of its predecessors (see the  $d$ -separation criteria in [5, 7, 3]). Formally we have  $(X_j \perp V_j | L \cup K)$ . By the contraction rule for conditional independencies (see [5]) the statements  $(X_j \perp V_j | L \cup K)$  and  $(X_j \perp L | K)$  imply  $(X_j \perp V_j | K)$ . Hence  $K$  must contain a set  $\mathbf{P}'_j$  that can be viewed as Markovian parents of  $X_j$ .

Now we can test whether a proper subset  $K'$  of  $K$  satisfies  $(X_j \perp L | K')$  and obtain a minimal set of parents of  $X_j$  by iterating this procedure.  $\square$

## 4 Learning the probabilities of $k$ -tuples

Now we shall present an upper bound on the required sample size in order to learn the probabilities of all  $k$ -tuples with good reliability. Then we can apply this result to the case  $k := 2\Delta + 1$ .

Let  $P(\cdot)$  be a probability distribution over an (ordered) set of random variables  $\mathbf{V} = \{X_1, \dots, X_n\}$  taking on values in  $\Omega_j$  for  $j = 1, \dots, n$ .

Let  $X_{j_1}, \dots, X_{j_k}$  be any  $k$ -subset of  $\mathbf{V}$ . We would like to have a reliable statement on the probability of the event  $(x_{j_1}, \dots, x_{j_k}) \in \Omega_{j_1} \times \dots \times \Omega_{j_k}$ , i.e. the probability

$$P(X_{j_1} = x_{j_1}, \dots, X_{j_k} = x_{j_k}). \quad (7)$$

The problem to determine the sample size required for estimating reliably the probability of *one specific* event is a usual problem of statistics. However, the problem we encounter in learning Bayesian networks is more sophisticated: we have to be almost sure that the estimated probabilities of all  $(2\Delta + 1)$ -tuples are sufficiently close to the real (unknown) probabilities.

The problem to determine whether and how fast the relative frequencies of a large set of events converge *uniformly* to their probabilities is well-known in statistical learning theory [8]. Statements on uniform convergence rely on the so-called Vapnik-Chervonenkis dimension (VC-dimension) of the considered set of events.

### Definition 5 (VC dimension)

Let  $P$  be an unknown probability measure on a probability space  $\Omega$  and  $S$  a set of events, i.e., a set of measurable subsets of  $\Omega$ . Define the VC-dimension of  $S := (M_\lambda)$  as the largest number  $h$  such that there exist  $h$  points  $\omega_1, \omega_2, \dots, \omega_h \in \Omega$  such that the sets  $M_\lambda \cap \{\omega_1, \dots, \omega_h\}$  run over all  $2^h$  subsets of  $\{\omega_1, \dots, \omega_h\}$ . Intuitively, one can consider the sets  $M_\lambda$  as classifiers and the VC-dimension as the largest number of points that can be classified in all  $2^h$  possible ways. The VC-dimension is said to be infinite if such an  $h$ -subset can be found for all  $h \in \mathbb{N}$ .

A trivial upper bound on the VC-dimension is given by the logarithm to base 2 of the number of events (in the case that  $S$  is finite).

Finite VC-dimension is known to be sufficient and necessary in order to have uniform convergence of relative frequencies to their probabilities. Quantitatively, one has the following theorem:

### Theorem 6 (Uniform convergence)

Let  $f(M)$  be the relative frequency of the number of occurrences of  $M$  after  $l$  runs. Let  $S$  have VC-dimension  $h$ . Let  $R_\epsilon$  be the risk (probability) that  $S$  contains at least one set  $M$  such that  $|f(M) - P(M)| \geq \epsilon$  for an arbitrary positive  $\epsilon$ . Then we have

$$R_\epsilon < 4 \exp \left\{ \left( \frac{h(1 + \ln(2l/h))}{l} - (\epsilon - 1/l)^2 \right) l \right\}. \quad (8)$$

**Proof:** see Theorem 4.4. in [8] □

This theorem allows to derive a lower bound on the required sample size in order to estimate the probability of all  $k$ -tuples. First we have to define the set of events and give an upper bound on its VC-dimension.

Let  $\Omega := \Omega_1 \times \dots \times \Omega_n$  be the probability space. This means that the  $j$ th random variable takes on values from  $\Omega_j$  for  $j = 1, \dots, n$ . The  $k$ -tuples are characterized by the positions and values the corresponding random variables take on. Let  $\mathbf{j} := \{j_1, j_2, \dots, j_k\}$  be an arbitrary  $k$ -subset of  $\{1, \dots, n\}$  and  $\mathbf{x} \in \Omega_{j_1}, \dots, \Omega_{j_k}$ .

We then denote by  $M_{\mathbf{x}}^{\mathbf{j}}$  the event that the random variables  $X_{j_1}, X_{j_2}, \dots, X_{j_k}$  take on the values  $x_{j_1}, \dots, x_{j_k}$ . This event corresponds uniquely to a cylinder set  $C_{\mathbf{x}}^{\mathbf{j}} \subset \Omega$ .

An upper bound on the VC-dimension of the set of those events that correspond to cylinder sets  $C_{\mathbf{x}}^{\mathbf{j}}$  is easy to get. Let  $d$  be the maximal cardinality of the sets  $\Omega_j$ . Then, for fixed  $k$ , there exist at most

$$d^k \binom{n}{k}$$

such cylinder sets. The first term gives an upper bound on the possible combinations of values and the second term the number of different positions. This number is smaller than  $(nd)^k$ . By taking the logarithm to base 2 we obtain an upper bound on the VC-dimension

$$h \leq k \log_2(nd) \tag{9}$$

Obviously, we can use much better bounds for concrete applications, e.g. given by Stirling's approximation (giving a less intuitive expression but providing a tighter bound). However, this crude upper bound is sufficient to study the asymptotic behavior.

Now we will present a lower bound on the VC-dimension in order to get an idea how tight the upper bound in (9) is.

We construct  $l$   $n$ -tuples with  $l := \lfloor \log_2(n - k + 1) \rfloor$  as follows. For each set  $\Omega_j$  we choose two different values  $x_{j,0}$  and  $x_{j,1}$  for  $j = 1, \dots, n$ . This defines a map  $\phi$  from the set of binary words of length  $n$  into  $\Omega$  by setting

$$\phi : b_1 b_2 \dots b_n \mapsto x_{1,b_1} x_{2,b_2} \dots x_{n,b_n} . \tag{10}$$

Now we define an  $l \times n$  matrix  $M$  with entries 0 and 1 as follows: The first  $k - 1$  columns have only 1 as entries. The next  $2^l$  columns are the binary words of length  $l$ . The remaining  $(n - k + 1 - 2^l)$  columns can be chosen arbitrarily.

The rows of  $M$  correspond to  $n$ -tuples by the map  $\phi$ . Let  $\mathcal{Y}$  be the set of those  $n$ -tuples and  $S$  be an arbitrary subset of  $\mathcal{Y}$ .  $S$  can uniquely be characterized by a vector  $s$  of length  $l$  with entries 0 and 1 where the  $j$ -th entry of  $s$  indicates whether the  $j$ -th  $n$ -tuple is an element of  $S$  or not. The matrix  $M$  contains a column that coincides

with  $s$ . Assume it to be the  $i$ -th column. Then  $C_{\mathbf{x}}^{\mathbf{j}} \cap \mathcal{Y}$  contains exactly those  $n$ -tuples that are elements of  $S$  provided that  $C_{\mathbf{x}}^{\mathbf{j}}$  is chosen as follows. Let  $\mathbf{j}$  be  $(1, 2, \dots, k-1, i)$  and choose  $\mathbf{x}$  as the  $k$ -tuple  $(x_{1;1}, x_{2;1}, \dots, x_{k-1;1}, x_{i;1})$ . This shows that the cylinder sets corresponding to  $k$ -tuples are able to classify  $\mathcal{Y}$  on all  $2^l$  possibilities. Therefore  $\lfloor \log_2(n-k+1) \rfloor$  is a lower bound on the VC-dimension of the cylinder sets. Comparing this bound with the upper bound in (9), we see that it gives the correct asymptotic behavior in the  $O$ -notation if  $k$  and  $d$  are considered as constants.

**Theorem 7** *For  $\epsilon > 0$  let  $R_\epsilon$  be the risk that there is a cylinder set  $C_{\mathbf{x}}^{\mathbf{j}}$  such that its relative frequency deviates from its probability by more than  $\epsilon$ . Then  $R_\epsilon$  can be made smaller than any  $\delta > 0$  while only increasing the sample size linearly with  $n$ .*

**Proof:** We choose  $l$  such that

$$\frac{l}{1 + \ln(2l)} \frac{(\epsilon - 1/l)^2}{2} \geq k \log_2(nd).$$

This can asymptotically be achieved by increasing  $l$  with  $O(n)$ , since  $l/(1 + \ln(2l)) \leq l/(\ln(l))$  and the latter term increases less than linearly in  $l$ .

Using our bound

$$h \leq k \log_2(nd)$$

we obtain

$$h \leq \frac{(\epsilon - 1/l)^2}{2} \frac{l}{1 + \ln(2l)}$$

and get

$$\frac{h(1 + \ln(2l))}{l} \leq \frac{(\epsilon - 1/l)^2}{2}.$$

By elementary calculation, this implies

$$\frac{h(1 + \ln(2l/h))}{l} - (\epsilon - 1/l)^2 \leq -\frac{(\epsilon - 1/l)^2}{2}.$$

Using the bound of Theorem 6 this shows that the risk  $R_\epsilon$  can even be made to decrease exponentially in  $n$  while increasing the sample size  $l$  only linearly in  $n$ .  $\square$

Note that the sample size has to be chosen such that the deviation of the relative frequencies from their probabilities is small compared to the relative frequencies. Then we have a reasonable criterion to decide for which sets  $\mathbf{X}, \mathbf{Y}, \mathbf{Z}$  of variables we may assume  $\mathbf{X}$  and  $\mathbf{Y}$  to be independent given  $\mathbf{Z}$ . This criterion is as follows: Based on the error bound of Theorem 6 we compute the relative uncertainty of the conditional probabilities used in the algorithm in the proof of Theorem 4. If the observed statistical dependencies are greater than the uncertainty we assume the variables to be dependent.



## 5 Conclusions

The sample size to learn the joint probability distribution on  $n$  nodes does only increase linearly with  $n$  if the underlying causal structure is assumed to be sufficiently simple. Here we considered the case that we know that the (unknown) causal graph has at most in-degree  $\Delta$  and a known time order exists. Then a graph that is Markov relative to the unknown probability measure can be found efficiently if only the probabilities of all  $(2\Delta + 1)$ -tuples are known. They can be learned with linear sample size. We have shown this by finding bounds on the VC-dimension of the corresponding cylinder sets. We would like to note that the causal structure can at least be *guessed* if only the probabilities of  $(2\Delta + 1)$ -tuples are known, since they allow to test a large number of statistical independencies.

## References

- [1] J. Cheng, D. Bell, and W. Liu. Learning belief networks from data: an information theory based approach. In *Proc. of the Sixth ACM International Conference on Information and Knowledge Management*, 1997.
- [2] N. Friedman, I. Nachman, and D. Peér. Learning bayesian network structure from massive datasets: The “sparse candidate” algorithm. In *Proc. Fifteenth Conf. on Uncertainty in Artificial Intelligence (UAI)*, 1999.
- [3] C. Glymour and G. F Cooper, editors. *Computation, Causation & Discovery*. AAAI Press/The MIT press, 1999.
- [4] J. Pearl. Bayesian networks: A model of self-activated memory for evidential reasoning. In *Proceedings, Cognitive Science Society*, pages 329–334, Greenwich, CT: Albex, 1985.
- [5] J. Pearl. *Probabilistic Reasoning in Intelligent Systems*. Morgan Kaufmann, San Mateo, CA, 1998.
- [6] J. Pearl. *Causality: models, reasoning, and inference*. Cambridge University Press, 2000.
- [7] P. Spirtes, C. Glymour, and R. Scheines. *Causation, Prediction, and Search*, volume 81 of *Lecture Notes in Statistics*. Springer, 1993.
- [8] V. N. Vapnik. *Statistical Learning theory*. Adaptive and learning systems for signal processing, communications, and control. Wiley Interscience, 1998.