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Blind Construction of Optimal Nonlinear Recursive Predictors for Discrete Sequences

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Abstract

We present a new method for nonlinear prediction of discrete random sequences under minimal structural assumptions. We give a mathematical construction for optimal predictors of such processes, in the form of hidden Markov models. We then describe an algorithm, CSSR (Causal-State Splitting Reconstruction), which approximates the ideal predictor from data. We discuss the reliability of CSSR, its data requirements, and its performance in simulations. Finally, we compare our approach to existing methods using variable-length Markov models and cross-validated hidden Markov models, and show theoretically and experimentally that our method delivers results superior to the former and at least comparable to the latter.

1 Introduction

The prediction of discrete sequential data is an important problem in many fields, including bioinformatics, neuroscience (spike trains), and nonlinear dynamics (symbolic dynamics). Existing prediction methods, with the exception of variable-length Markov model (VLMM) methods, make strong assumptions about the nature of the data-generating process. In this paper, we present an algorithm for the blind construction of asymptotically optimal nonlinear predictors of discrete sequences. These predictors take the form of minimal sufficient statistics, naturally arranged into a hidden Markov model (HMM). We thus secure the many desirable features of HMMs, and hidden-state models more generally, without having to make *a priori* assumptions about the architecture of the system. Furthermore, our method is more widely applicable than those based on VLMMs. We also compare our approach to the use of cross-validation to select an HMM architecture, and find our results are at least comparable in terms of accuracy and parsimony, and superior in terms of speed. For reasons of space, we omit proofs here. These can be found in [1, ch. 5] and [2]. The source code and documentation for an implementation of CSSR are at `http://bactra.org/CSSR/`.

2 Optimal Nonlinear Predictors

Consider a sequence of random variables X_t drawn from a discrete alphabet $\mathcal{A}$. A predictive *statistic* is a function η on the past measurements $X_{-\infty}^{t}$. We want to predict the process, so we want the statistic to summarize the information $X_{-\infty}^{t}$ contains about X_{t+1}^{∞}. That is, we wish to maximize the mutual information between the statistic $\eta(X_{-\infty}^{t})$ and the future X_{t+1}^{∞}, i.e., in the standard notation, maximize $I[\eta(X_{-\infty}^{t}); X_{t+1}^{\infty}]$, which can be at most $I[X_{-\infty}^{t}; X_{t+1}^{\infty}]$. A *sufficient* statistic is one which reaches this level. This implies η is sufficient if and only if $\eta(x^-) = \eta(y^-)$ implies $\mathrm{P}(X_{t+1}^{\infty}|X_{-\infty}^{t} = x^-) = \mathrm{P}(X_{t+1}^{\infty}|X_{-\infty}^{t} = y^-)$ [3]. Decision theory shows that optimal prediction requires only knowledge of a sufficient statistic [4]. It is desirable to compress a sufficient statistic, so as to minimize the information needed for optimal prediction. One sufficient statistic η_1 is smaller than another η_2 if η_1 can be calculated from η_2. A *minimal* sufficient statistic is one which can be calculated from any other sufficient statistic. Minimal sufficient statistics thus are the most compact summary of the data which retains all the predictively-relevant information. We now construct one, following [5] and [6].

Say that two histories x^- and y^-, are equivalent when $\mathrm{P}(X_{t+1}^{\infty}|X_{-\infty}^{t} = x^-) = \mathrm{P}(X_{t+1}^{\infty}|X_{-\infty}^{t} = y^-)$. The equivalence class of x^- is $[x^-]$. Define the function which maps histories to their equivalence classes:

$$\epsilon(x^-) \equiv [x^-]$$
$$= \left\{y^- : \mathrm{P}(X_{t+1}^{\infty}|X_{-\infty}^{t} = y^-) = \mathrm{P}(X_{t+1}^{\infty}|X_{-\infty}^{t} = x^-)\right\}$$

The possible values of ϵ, i.e., the equivalence classes, are known as the "causal states" of the process; each corresponds to a distinct distribution for the future. (We comment on the name "causal state" below.) The state at time t is $S_t = \epsilon(X_{-\infty}^{t})$. Clearly, $\epsilon(x^-)$ is a sufficient statistic. It is also minimal, since if η is sufficient, then $\eta(x^-) = \eta(y^-)$ implies $\epsilon(x^-) = \epsilon(y^-)$. One can further show [6] that ϵ is the *unique* minimal sufficient statistic, meaning that any other must be isomorphic to it.

The causal states have some important properties [6]. (1) $\{S_t\}$ is a Markov process. (2) The causal states are recursively calculable; there is a function T such that $S_{t+1} = T(S_t, X_{t+1})$. (3) One can represent the observed process X as a random function of the causal state process, i.e., there is naturally a hidden-Markov-model representation. (The familiar correspondence between HMMs and state machines lets us re-phrase the second property as: the causal states form a deterministic machine.) We will refer to *causal state models* or *causal state machines.*

The construction of the causal states is essentially the same as that of the "measure-theoretic prediction process" introduced by Frank Knight [7], though that is framed directly in terms of the conditional distributions. Both can be regarded as applications of Wesley Salmon's concept of a "statistical relevance basis" [8] to time series. Causal states are also closely related to the "predictive state representations" (PSRs) of controlled dynamical systems due to Littman, Sutton and Singh [9], though PSRs are not generally minimal. (There is currently no discovery procedure for PSRs, though there are ways to learn the parameters of a *given* PSR [10].) It is not clear that the "causal states" really are causal in the strong sense of e.g. [11], but this needs investigation. Meanwhile, they need a name, and "causal states" is less awkward than the others.

Our algorithm for inferring the causal states from data builds on the following observation [6, pp. 842–843]. Say that η is *next-step sufficient* if $I[X_{t+1}; \eta(X_{-\infty}^t)] = I[X_{t+1}; X_{-\infty}^t]$. A next-step sufficient statistic contains all the information needed for optimal one-step-ahead prediction, but not necessarily for longer predictions. If η is next-step sufficient, and it is recursively calculable, then η is sufficient for the whole of the future. Since ϵ satisfies these hypotheses, the minimal sufficient statistic can be found by searching among those which are next-step sufficient and recursive.

3 Causal-State Splitting Reconstruction

We now describe an algorithm, Causal-State Splitting Reconstruction (CSSR), that estimates an HMM with the properties described in the last section from sequence data. CSSR starts by "assuming" the process is an independent, identically-distributed sequence, with one causal state, and adds states when statistical tests show that the current set of states is not sufficient.

Suppose we are given a sequence $\bar{x}$ of length N from a finite alphabet $\mathcal{A}$ of size k. We wish to derive from this an estimate $\hat{\epsilon}$ of the the minimal sufficient statistic ϵ. We will do this by finding a set of states Σ, each member of which will be a set of strings, or finite-length histories. The function $\hat{\epsilon}$ will then map a history x^- to whichever state contains a suffix of x^- (taking "suffix" in the usual string-manipulation sense). Although each state can contain multiple suffixes, one can check [2] that the mapping $\hat{\epsilon}$ will never be ambiguous. (This contrasts with the variable-length Markov models described in Sec. 5.1 below, where each state contains only a single suffix.)

The *null hypothesis* is that the process is Markovian on the basis of the states in Σ; that is,

$$\mathrm{P}(X_t | X_{t-L}^{t-1} = a x_{t-L+1}^{t-1}) = \mathrm{P}(X_t | \hat{S} = \hat{\epsilon}(x_{t-L+1}^{t-1})) \quad (1)$$

for all $a \in \mathcal{A}$. That is, adding an additional piece of history does not change the conditional distribution for the next observation. We can check this with a standard statistical test, such as χ^2 or Kolmogorov-Smirnov (which we used in our experiments below). If we reject this hypothesis, we fall back on a *restricted alternative hypothesis*, which is that we have the right set of conditional distributions, but have matched them with the wrong histories. That is,

$$\mathrm{P}(X_t | X_{t-L}^{t-1} = a x_{t-L+1}^{t-1}) = \mathrm{P}(X_t | \hat{S} = s^*) \quad (2)$$

for some $s^* \in \Sigma$, but $s^* \neq \hat{\epsilon}(x_{t-L+1}^{t-1})$. If this hypothesis passes a statistical test, again with size α, then s^* is the state to which we assign the history[1]. Only if the restricted alternative is itself rejected do we create a new state, with the suffix $a x_{t-L+1}^{t-1}$.

The algorithm itself has three phases; pseudo-code is given in Figure 1. Phase I initializes Σ to a single state, which contains only the null suffix $\emptyset$. (That is, $\emptyset$ is a suffix of any string.) The length of the longest suffix in Σ is L; this starts at 0. Phase II iteratively tests the successive versions of the null hypothesis, Eq. 1, and L increases by one each iteration, until we reach some maximum length $L_{\max}$. At the end of II, $\hat{\epsilon}$ is (approximately) next-step sufficient. Phase III makes $\hat{\epsilon}$ recursively calculable, by splitting the states until they have deterministic transitions. The last phase is not as straightforward as it may seem.

[1] If more than one such state s^* exists, we chose the one for which $\widehat{\mathrm{P}}(X_t | \hat{S} = s^*)$ differs least, in total variation distance, from $\widehat{\mathrm{P}}(X_t | X_{t-L}^{t-1} = a x_{t-L+1}^{t-1})$, which is plausible and convenient. However, which state we chose is irrelevant in the limit $N \to \infty$, so long as the difference between the distributions is not statistically significant.

There are standard algorithms [12] to take a non-deterministic finite automaton (NDFA) and produce a deterministic finite automaton (DFA), which is equivalent in the sense of generating the same language. However, these algorithms do not ensure that each state of the DFA, considered as an equivalence class of strings, is a subset of a state of the NDFA. In the present context, applying one of these algorithms would result in states which mixed histories with significantly different conditional distributions for the next symbol — we would get a statistic which was recursive but *not* next-step sufficient. To preserve probabilistic information while making the transitions deterministic, we proceed as follows [2]. We want there to be a transition function $T(s, b)$ such that $\hat{\epsilon}(x^{-}b) = T(s, b)$ for any $x^{-} \in s$. Thus, for each state-symbol pair s, b, we check whether $\hat{\epsilon}(x^{-}b)$ is the same for all $x^{-} \in s$. If we find a state-symbol pair where this does not hold, we split that state into states where it does hold. We then start checking the state-symbol pairs all over again, since some other transitions may have been altered. This procedure always terminates, leaving us with a set of states with deterministic transitions. To do this smoothly, we must first remove any transient states which the second phase may have created. These transients are never true causal states [13], but are sometimes useful in filtering applications, in which case they can be straightforwardly restored from the true, recurrent states [13].

$\widehat{\mathrm{P}}(X_t | X_{t-L}^{t-1} = x)$ may be estimated in several ways; we have used simple maximum likelihood. $\widehat{\mathrm{P}}(X_t | \hat{S} = s)$, in turn, must be estimated, and we used the weighted average of the estimated distributions of the histories in s. When $L = 0$ and the only state contains just the null string, $\widehat{\mathrm{P}}(X_t | \hat{S} = s) = \widehat{\mathrm{P}}(X_t)$, the unconditional probability distribution.

3.1 Time Complexity

Phase I computes the relative frequency of all words in the data stream, up to length $L_{\max} + 1$. There are several ways this can be done using just a single pass through the data. In our implementation, as we scan the data, we construct a parse tree which counts the occurrences of all strings whose length does not exceed $L_{\max} + 1$. Thereafter we need only refer to the parse tree, not the data. This procedure is therefore $O(N)$, and this is the only sub-procedure whose time depends on N.

Phase II checks, for each suffix ax, whether it belongs to the same state as its parent x. Using a hash table, we can do this, along with assigning ax to the appropriate state, creating the latter if need be, in constant time. Since there are at most $u(k, L_{\max}) \equiv$

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Algorithm CSSR($\mathcal{A}$,$\bar{x}$, $L_{\max}$, $\alpha$)
I. Initialization: $L \leftarrow 0$, $\Sigma \leftarrow \{\{\emptyset\}\}$
II. Sufficiency:
  while $L < L_{\max}$
      for each $s \in \Sigma$
          estimate $\widehat{\mathrm{P}}(X_t | \hat{S} = s)$
          for each $x \in s$
              for each $a \in \mathcal{A}$
                  estimate $p \leftarrow \widehat{\mathrm{P}}(X_t | X_{t-L}^{t-1} = ax)$
                  Test($\Sigma, p, ax, s, \alpha$)
      $L \leftarrow L + 1$
III. Recursion:
    Remove transient states from $\Sigma$
    recursive ← False
    until recursive
        recursive ← True
        for each $s \in \Sigma$
            for each $b \in \mathcal{A}$
                $x_0 \leftarrow$ first $x \in s$
                $T(s, b) \leftarrow \hat{\epsilon}(x_0 b)$
                for each $x \in s$, $x \neq x_0$
                    if $\hat{\epsilon}(xb) \neq T(s, b)$
                    then create new state $s' \in \Sigma$
                        $T(s', b) \leftarrow \hat{\epsilon}(xb)$
                        for each $y \in s$ such that
                                $\hat{\epsilon}(yb) = \hat{\epsilon}(xb)$
                            Move($y, s, s'$)
                        recursive ← False

Test($\Sigma, p, ax, s, \alpha$)
    if null hypothesis (Eq. 1) passes a test of size $\alpha$
    then $s \leftarrow ax \cup s$
    else if restricted alternative hypothesis (Eq. 2)
            passes a test of size $\alpha$ for $s^* \in \Sigma$, $s^* \neq s$
    then Move($ax, s, s^*$)
    else create new state $s' \in \Sigma$
        Move($ax, s, s'$)

Move($x, s_1, s_2$)
    $s_1 \leftarrow s_1 \setminus x$
    re-estimate $\widehat{\mathrm{P}}(X_t | \hat{S} = s_1)$
    $s_2 \leftarrow s_2 \cup x$
    re-estimate $\widehat{\mathrm{P}}(X_t | \hat{S} = s_2)$
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Figure 1: Pseudo-code for the algorithm CSSR. Arguments: $\mathcal{A}$: discrete alphabet for the stochastic process; $\bar{x}$: sequence of length N drawn from $\mathcal{A}$; $L_{\max}$, maximum history length considered when estimating causal states; α, size of the hypothesis tests, i.e., probability of falsely rejecting the hypothesis being tested. Newly created states are always empty initially.

$(k^{L_{\max}+1}-1)/(k-1)$ suffixes, the time for phase II is $O(u(k, L_{\max})) = O(k^{L_{\max}})$.

Phase III itself has three parts: getting the transition structure, removing transient states, and refining the states until they have recursive transitions. The time to find the transition structure is at most $ku(k, L_{\max})$. Removing transients can be done by finding the strongly-connected components of the state-transition graph, and then finding the recurrent part of the connected-components graph. Both these operations take a time proportional to the number of nodes plus the number of edges in the state-transition graph. The number of nodes in the latter is at most $u(k, L_{\max})$, since there must be at least one suffix per node, and there are at most k edges per node. Hence transient-removal is $O(u(k, L_{\max})(k+1)) = O(k^{L_{\max}+1} + k^{L_{\max}}) = O(k^{L_{\max}+1})$. As for refining the states, the time needed to make one refining pass is $ku(k, L_{\max})$, and the maximum number of passes needed is $u(k, L_{\max})$, since, in the worst case, we will have to make every suffix its own state, and do so one suffix at a time. So the maximum time for refinement is $O(ku^2(k, L_{\max})) = O(k^{2L_{\max}+1})$, and the maximum time for all of phase III is $O(k^{L_{\max}+1} + k^{L_{\max}+1} + k^{2L_{\max}+1}) = O(k^{2L_{\max}+1})$. Note that if removing transients consumes the maximal amount of time, then refinement cannot and vice versa.

Adding up, and dropping lower-order terms, the total time complexity for CSSR is $O(k^{2L_{\max}+1}) + O(N)$. Observe that this is linear in the data size N. The high exponent in k is reached only in extreme cases, when every string spawns its own state, almost all of which are transient, etc. In practice, we have found CSSR to be much faster than this worst-case result suggests[2].

4 Convergence and Performance

We have established the convergence of CSSR on the correct set of states, subject to suitable conditions. The proofs, which use large deviations theory on Markov chains, are too long to give here, so we simply state the assumptions and the conclusions [2].

We make the following hypotheses.

1. The process is conditionally stationary. That is, for all values of τ, $\mathrm{P}(X_{t+1}^{\infty} | X_{-\infty}^{t} = x^-) = \mathrm{P}(X_{t+\tau+1}^{\infty} | X_{-\infty}^{t+\tau} = x^-)$.
2. The process has only finitely many causal states.
3. Every state contains at least one suffix of finite length. That is, there is some Λ such that every state contains a suffix of length Λ or less. This does not mean that Λ symbols of history always fix the state, just that it is *possible* to synchronize [13] to every state after seeing no more than Λ symbols.

Under these assumptions, the reconstructed set of causal states "converges in probability" on the true causal states, in the sense that

$$\mathrm{P}(\exists x^- : \epsilon(x^-) \neq \hat{\epsilon}(x^-)) \to 0$$

as $N \to \infty$ [2, p. 16]. We establish this by showing that the probability of assigning a history to the wrong equivalence class goes to zero as $N \to \infty$. More exactly, for a pair of histories x^-, y^-, define the events

$$\begin{aligned} E(x^-, y^-) &\equiv (\hat{\epsilon}(x^-) = \hat{\epsilon}(y^-)) \wedge (\epsilon(x^-) \neq \epsilon(y^-)), \\ F(x^-, y^-) &\equiv (\hat{\epsilon}(x^-) \neq \hat{\epsilon}(y^-)) \wedge (\epsilon(x^-) = \epsilon(y^-)) \ . \end{aligned}$$

Then [2, pp. 15–16]

$$\forall x^-, y^-, \ \mathrm{P}(E(x^-, y^-) \cup F(x^-, y^-)) \to 0 \ .$$

To establish this fact in its turn, we use large deviation theory for Markov chains to show that the empirical conditional distribution for each history converges on its true value exponentially quickly [2, pp. 12–13], and consequently the probability that any of our estimated conditional distributions differs significantly from its true value goes to zero exponentially in N [2, pp. 13–15]. The test size α does not affect this convergence, becoming irrelevant in the limit of large N. (With finite N, of course, α influences our risk of making states simply on the basis of sampling fluctuations.) Under some further assumptions, $\mathrm{P}(\hat{\epsilon} \neq \epsilon)$ actually goes to zero exponentially in N, and then, by the Borel-Cantelli Lemma, one has the wrong structure only finitely often before converging on the true causal states.

If the states are correct, then another large-deviation argument [2, sec. 4.3] gives us a handle on the expected prediction error. Since the forecasts made by our predictors are distributional, error should be measured as a divergence between the predicted distribution and the true one. Using the total variation metric[3] as our divergence measure, error goes down as $N^{-1/2}$. This is illustrated in Figure 5.

[2] Average-case time complexity will depend on the statistical properties of the data source. For instance, the number of strings of length $L_{\max}$ is here bounded by $u(k, L_{\max}) \approx k^{L_{\max}}$. But if $L_{\max}$ is reasonably large, and the source satisfies the asymptotic equipartition property [14, sec. 15.7], only $\approx 2^{hL_{\max}}$ strings are produced with positive probability, where $h \leq \log k$ is the source entropy rate.

[3] The total variation or L_1 distance between two measures P and Q over a discrete space $\mathcal{A}$ is $d(P,Q) \equiv \sum_{a \in \mathcal{A}} |P(a) - Q(a)|$. Scheffe's identity [15] asserts that $d(P,Q) = 2 \sup_{\mathrm{A} \subseteq \mathcal{A}} |P(\mathrm{A}) - Q(\mathrm{A})|$, and consequently $0 \leq d(P,Q) \leq 2$.

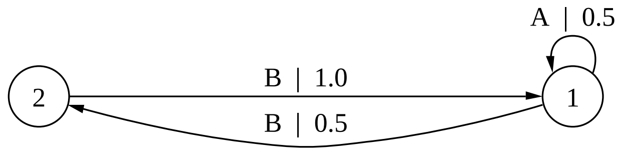

Figure 2: The Even Process. Transition labels show the symbol emitted, and the probability of making the transition.

Of the three assumptions in our convergence proof, the only one which affects the parameters of the algorithm is the third, that there is an integer Λ such that each of the true causal states contains at least one suffix of length Λ or less. Λ is thus a characteristic of the underlying process, not CSSR. If $L_{\max} < \Lambda$, not only does the proof of convergence fail, there is no way to obtain the true states. For periodic processes Λ is equal to the period; there are no general results for other kinds of processes.

Rather than guessing Λ, one might use the largest feasible $L_{\max}$, but this is limited by the quantity of data [17]. Let $L(N)$ be the the maximum L we can use when we have N data-points. If the observed process has the weak Bernoulli property (which random functions of irreducible Markov chains do), and an entropy rate of h, then a sufficient condition for the convergence of sequence probability estimates is that $L(N) \leq \log N/(h+\varepsilon)$, for some positive ε. If $L(N) \geq \log N/h$, probability estimates over length L words do not converge. We must know h to use this result, but $\log k \geq h$, so using $\log k$ in those formulas gives conservative estimates. For a given process and data-set, it is of course possible that $L(N) < \Lambda$, in which case we simply haven't enough data to reconstruct the true states.

We have tested CSSR on a variety of real and simulated data sources, and here report two simulated examples, both binary-valued: the "even process," illustrated in Figure 2, and a seven-state process used in experimental studies of human sequence prediction [16], illustrated in figure 3. (The results of applying CSSR to neuronal spike trains will be reported elsewhere.)

For the even process, the system can start in either state 1 or state 2. When in state 1 it is equally likely to emit an A, staying in 1, or emit a B, moving to 2. In 2 it always emits a B and moves to 1. This is an HMM, but it is not equivalent to any finite-order Markov chain (see below). Figures 4 and 5 illustrate the ability of CSSR to get the correct number of causal states, the correct transition structure, and the correct distributions. Figure 5 also shows the asymptotic scaling of the error with N. Curves average over 30 independent trials at each N; α is fixed to 10^{-3}. Results for the seven-state process of Figure 3 are given in Section 5.2.

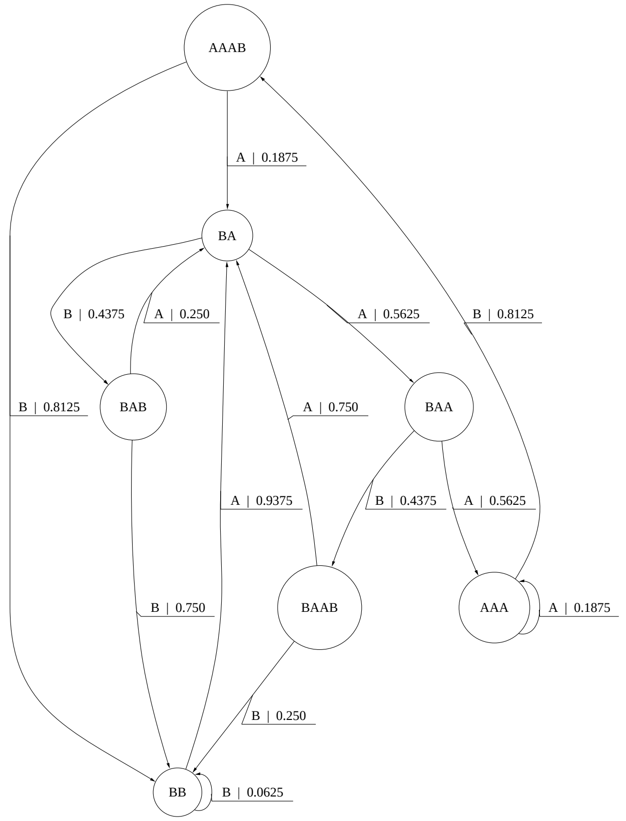

Figure 3: A seven-state process, used in [16] to study human sequence prediction. Here each state is defined by a single suffix, as indicated. All transition probabilities are multiples of 1/16.

5 Comparison with Previous Methods

5.1 Variable-Length Markov Models

The "context" algorithm of Rissanen [18] and its descendants [19, 20, 21, 22] construct "variable-length Markov models" (VLMMs) from sequence data. They find a set of *contexts* such that, given the context, the past of the sequence and its next symbol are conditionally independent. Contexts are taken to be suffixes of the history, and the algorithms work by examining increasingly long histories, creating new contexts by splitting existing ones into longer suffixes when thresholds of error are exceeded [23]. (This means that contexts can be arranged in a tree, so these are also called "context tree" or "probabilistic suffix tree" [23] algorithms.)

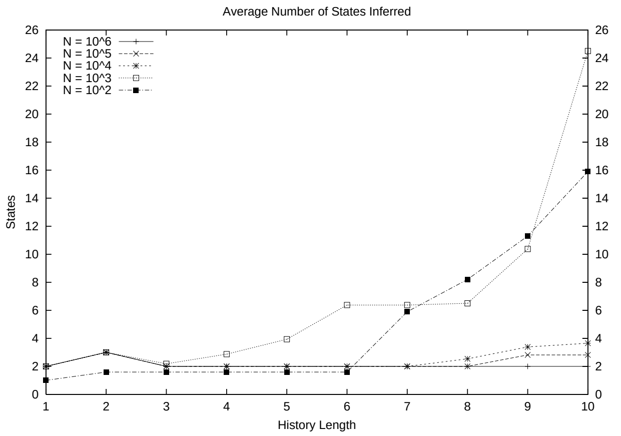

Figure 4: Number of states inferred versus $L_{\max}$ and N for the even process. The true number of causal states is 2.

Causal state reconstruction has an important advantage over VLMM methods. Each state in a VLMM is represented by a single suffix, and consists of all and only the histories ending in that suffix. For many processes, the causal states contain multiple suffixes. In these cases, multiple "contexts" are needed to represent a single causal state, so VLMMs are generally more complicated than the HMMs we build. The causal state model is the same as the minimal VLMM if and only if every causal state contains a *single* suffix. This is the case for the process in Fig. 3, where CSSR and VLMM methods will give the same results.

Recall the even process of the last section. Any history ending in A, or in an A followed by an even number of B's, belongs to state 1. Any history terminated by an A followed by an odd number of B's, belongs to 2. Clearly 1 and 2 both contain infinitely many suffixes, and so correspond to an infinite number of contexts. VLMMs are simply incapable of capturing this structure. If we let $L_{\max}$ grow, a VLMM algorithm will increase the number of contexts it finds without bound, but cannot achieve the same combination of predictive power and model simplicity as causal state reconstruction (as illustrated by Figures 4 and 5). Note, too, that the causal states for the even process have finite representations, even though they contain infinitely many suffixes.

The even process is one of the *strictly sofic processes* [24, 25], which can be described by finite state models, but are not Markov chains of any finite order[4]. Just as VLMMs cannot handle the even process, they cannot handle any strictly sofic process, even though those are just regular languages. Causal states cannot provide a finite representation of every stochastic regular language [13], but the class they capture strictly includes those captured by VLMMs.

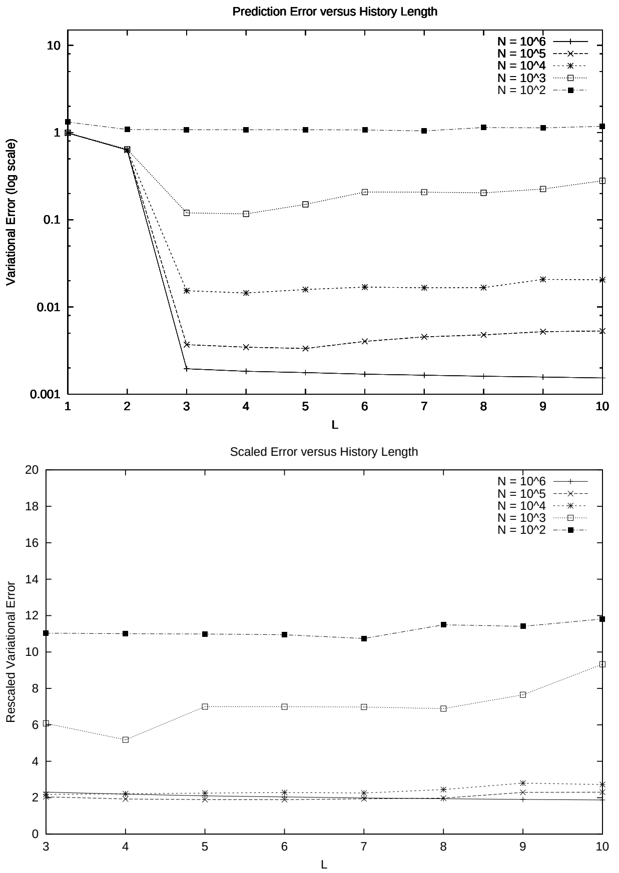

Figure 5: Prediction error as a function of $L_{\max}$ and N for the even process. Error is the total-variation distance between the actual distribution over words of length 10, and that predicted by the inferred states. Top panel: error (log scale) as a function of $L_{\max}$. Bottom: error times $\sqrt{N}$ (linear scale). Here $3 \leq L_{\max} \leq 10$, since if $L_{\max} < 3$ CSSR cannot find the correct states. With this α, CSSR never gets the states right for $N = 10^2$, and only sporadically for $N = 10^3$, so those lines are not on the scaling curve.

5.2 Cross-Validation

A standard heuristic for finding the right HMM architecture is cross-validation [26]. One picks multiple candidate architectures, training each one using the expectation-maximization (EM) algorithm, and then compares their performance on fresh test data, selecting the one with the smallest out-of-sample error.

To compare the performance of CSSR against this baseline, we started with fully-connected HMMs with

[4] More exactly, each history x^- has a *follower set* of futures x^+ which can succeed it. A process is *sofic* if it has only a finite number of distinct follower sets, and strictly sofic if it is sofic and has an infinite number of irreducible forbidden words.

N	d_{CV}	d_{CSSR}	$\hat{s}_{CV}$	$\hat{s}_{CSSR}$
10^2	1.27 ± 0.23	1.10 ± 0.23	6.6 ± 1.5	1.6 ± 1.0
10^3	1.25 ± 0.41	0.19 ± 0.23	5.6 ± 1.7	2.2 ± 0.1
10^4	1.15 ± 0.02	0.02 ± 0.02	2.0 ± 0	2.0 ± 0

Table 1: Comparison of the performance of HMM cross-validation to CSSR on the even process. d_{CV}, total-variation distance between cross-validated HMM and the even process; d_{CSSR}, distance between reconstructed causal state model and the even process; $\hat{s}_{CV}$, number of states in cross-validated HMM; $\hat{s}_{CSSR}$, number of states in reconstructed model. In all cases the numbers given are the means over multiple independent trials, plus or minus one standard deviation. Recall that $0 \leq d \leq 2$, and that the minimal number of states needed is 2.

M states, $M = 1$ to 10. We trained these, using the EM algorithm, on N data-points from the even process. Our test data consisted of another N data-points from an independent realization, and we selected HMMs based on the log-likelihood they assigned to the test data. Following common practice, the initial HMM parameters fed to the EM algorithm were those for fully-connected models, i.e., every state could transition to every other state, and every state could emit every symbol. We then calculated, for each cross-validated HMM, the total variation distance between the distributions it and the even process generated over sequences of length 10. (Because cross-validation is so computationally intensive, we have only compared up to length $N = 10^4$.) Table 1 compares this error measure for the cross-validated HMMs and for the reconstructed causal state models. It also indicates the number of states selected by cross-validation, which is consistently higher than the number needed by CSSR. Table 2 gives the results of a completely parallel procedure applied to the seven-state process.

CSSR, like the VLMM methods, is a constructive approach. Cross-validation is not constructive but selective. In our case, starting with fully-connected models (which, again, is a standard heuristic), cross-validated expectation-maximization *never* selected a model whose structure corresponded to the minimal sufficient statistic of the data-generating process. In both cases, the generalization of HMMs with more states worsened as the data-length grew, so cross-validation increasingly favored small HMMs which, while bad predictors, at least did not over-fit. Had models with the correct structure been in the initial population of candidates, they doubtless would have done quite well, and the gap in predictive performance between CSSR and cross-validation would be much smaller. Even when we have such prior architectural knowledge, CSSR will typically be faster than cross-validated EM, which involves performing nonlinear optimization on multiple model structures.

N	d_{CV}	d_{CSSR}	$\hat{s}_{CV}$	$\hat{s}_{CSSR}$
10^2	1.41 ± 0.23	0.70 ± 0.12	4.5 ± 2.1	5.1 ± 1.5
10^3	1.40 ± 0.17	0.21 ± 0.06	5.8 ± 2.7	6.6 ± 0.8
10^4	1.40 ± 0.11	0.06 ± 0.01	2.3 ± 0.7	7.2 ± 0.6

Table 2: Comparison of the performance of HMM cross-validation to CSSR on the seven-state process. Variables are as in 1.

6 Conclusion

We have described an algorithm, CSSR, for the unsupervised construction of optimal nonlinear predictors of discrete sequences. The predictors take the form of minimal sufficient statistics, arranged naturally into a hidden Markov model. CSSR's time complexity is linear in the data size. It reliably infers the statistical structure of processes with finitely many causal states. CSSR's predictive performance is at least comparable to cross-validated expectation-maximization, but it is constructive and faster; and the class of processes it can represent is strictly larger than those of competing constructive methods, such as variable-length Markov models.

Two directions for future work suggest themselves. (1) CSSR does not *require* prior knowledge about system dynamics, but by the same token cannot exploit such knowledge when it exists. One way around this would be to initialize the algorithm with a non-trivial partition of histories, reflecting a guess about which patterns are dynamically important, and let CSSR revise that partition the way it does now. It would be interesting to know when CSSR could correct an erroneous initial partition. (2) HMMs are models of dynamical systems without inputs. Partially-observable Markov decision processes (POMDPs) model systems with inputs, i.e., controlled dynamical systems. The causal state theory we have used generalizes naturally to this setting [1, ch. 7], where it is especially closely connected to PSRs. Suffix-tree methods can induce POMDPs from data [23, 27, 28], and we believe CSSR can be adapted to reconstruct POMDPs. This would provide a discovery procedure for PSRs.

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