Causality Networks

Ishanu Chattopadhyay
ic99@cornell.edu

Abstract—While correlation measures are used to discern statistical relationships between observed variables in almost all branches of data-driven scientific inquiry, what we are really interested in is the existence of causal dependence. Statistical tests for causality, it turns out, are significantly harder to construct; the difficulty stemming from both philosophical hurdles in making precise the notion of causality, and the practical issue of obtaining an operational procedure from a philosophically sound definition. In particular, designing an efficient causality test, that may be carried out in the absence of restrictive pre-suppositions on the underlying dynamical structure of the data at hand, is non-trivial. Nevertheless, ability to computationally infer statistical prima facie evidence of causal dependence may yield a far more discriminative tool for data analysis compared to the calculation of simple correlations. In the present work, we present a new non-parametric test of Granger causality for quantized or symbolic data streams generated by ergodic stationary sources. In contrast to state-of-art binary tests, our approach makes precise and computes the degree of causal dependence between data streams, without making any restrictive assumptions, linearity or otherwise. Additionally, without any a priori imposition of specific dynamical structure, we infer explicit generative models of causal cross-dependence, which may be then used for prediction. These explicit models are represented as generalized probabilistic automata, referred to crossed automata, and are shown to be sufficient to capture a fairly general class of causal dependence. The proposed algorithms are computationally efficient in the PAC sense; i.e., we find good models of cross-dependence with high probability, with polynomial run-times and sample complexities. The theoretical results are applied to weekly search-frequency data from Google Trends API for a chosen set of socially "charged" keywords. The causality network inferred from this dataset reveals, quite expectedly, the causal importance of certain keywords. It is also illustrated that correlation analysis fails to gather such insight.

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1 Motivation

“Causation does not imply causation” is a lesson taught early and often in statistics. The obvious next question is almost always left untouched by the preliminary texts: how do we then test for causality? This is an old question debated in philosophy [1], [2], [3], [4], [5], law [6], statistics [7], [8], [9], [10], and more recently, in learning theory; with experts largely failing to agree on a philosophically sound operational approach. Causality, as an intuitive notion, is not hard to grasp. The lack of consensus on how to infer causal relationships from data is perhaps ascribable to the difficulty in making this intuitive notion mathematically precise.

“Unlike art, causality is a concept (for) whose definition people know what they do not like, but few know what they do like.”

- C.W.J. Granger [11]
Granger’s attempt at obtaining a precise definition of causal influence proceeds with the setting up of a framework sufficiently general for statistical discourse: Consider a universe in which variables are measured at pre-specified time points \( t = 1, 2, \cdots \). Denote all available knowledge in the universe up to time \( n \) as \( \Omega_{\infty} \), and let \( \Omega_{\infty} \setminus Y_{\infty} \) denote this complete information except the values taken by a variable \( Y \) up to time \( n \), where \( Y_{\infty} \in \Omega_{\infty} \). \( \Omega_{\infty} \) includes no variates measured at time points \( t > n \), although it may well contain expectations or forecasts of such values. However, these expectations will simply be functions of \( \Omega_{\infty} \). We need additional structure before we define causality, namely:

- **Axiom A**: The past and present may cause the future, but the future cannot cause the past.
- **Axiom B**: \( \Omega_{\infty} \) contains no redundant information, so that if some variable \( Z \) is functionally related to one or more other variables, in a deterministic fashion, then \( Z_{\infty} \) should be excluded from \( \Omega_{\infty} \).

Within this framework, Granger suggests the following definition, noting that it is not effective [12], i.e., not directly applicable to data:

**Definition 1** (Granger Causality). \( Y_{\infty} \) is said to cause \( X_{\infty} \) if given a set \( A \) in which the variable \( X_{\infty} \) takes values in, we have:

\[
Pr(X_{n+1} \in A|\Omega_{\infty}) \neq Pr(X_{n+1} \in A|\Omega_{\infty} \setminus Y_{\infty})
\]  

(1)

Granger’s notion is intuitively simple: \( Y \) is a cause of \( X \), if it has unique information that alters the probabilistic estimate of the immediate future of \( X \). Not all notions of causal influence are expressible in this manner, neither can all philosophical subtleties be adequately addressed. Granger’s motivation was more pragmatic - he was primarily interested in obtaining a mathematically precise framework that leads to an effective or algorithmic solution - a concrete statistical test for causality.

### 1.1 Granger’s Operational Definitions of Causality

Short of encoding “all knowledge” in the universe up to a given time point, Definition 1 is not directly useful. Suppose that one is interested in the possibility that a vector series \( Y_t \) causes another vector \( X_t \). Let \( J_n \) be an information set available at time \( n \), consisting of terms of the vector series \( Z_t \), i.e.,

\[
J_n = \{ Z_t : t \leq n \}
\]  

(2)

\( J_n \) is said to be a proper information set with respect to \( X_t \), if \( X_t \) is included within \( Z_t \). Further, suppose that \( Z_t \) does not include any component of \( Y_t \), and define

\[
J'_n = \{ (Z_t, Y_t) : t \leq n \}
\]  

(3)

Denote by \( F(X_{n+1}|J_n) \) the conditional distribution function of \( X_{n+1} \) given \( J_n \), and define:

**Definition 2**. \( Y_t \) does not cause \( X_{\infty} \) with respect to \( J_n \) if:

\[
F(X_{n+1}|J_n) = F(X_{n+1}|J'_n)
\]  

(4)

i.e., the extra information in \( J'_n \) has not affected the conditional distribution. A necessary condition is that:

\[
E(X_{n+1}|J_n) = E(X_{n+1}|J'_n)
\]  

(5)

- **If** \( J'_n = \Omega_{\infty} \), the universal information set, and if

\[
F(X_{n+1}|J_n) \neq F(X_{n+1}|J'_n)
\]  

(6)

then, \( Y_n \) is said to cause \( Y_{\infty} \).

- \( Y_n \) is a prima facie cause of \( X_{\infty} \) with respect to \( J_n \) if:

\[
F(X_{n+1}|J_n) \neq F(X_{n+1}|J'_n)
\]  

(7)

- \( Y_n \) is said not to cause \( X_{\infty} \) in the mean with respect to \( J_n \) if:

\[
\Delta(J_n) = E(X_{n+1}|J_n) - E(X_{n+1}|J_n) = 0
\]  

(8)

- If \( \Delta(J_n) \) is not identically zero, then \( Y_n \) is a prima facie cause of \( X_{\infty} \) in the mean with respect to \( J_n \).

**Definition 2** is far more useful; with a little more structure we may obtain an effective causality test. We will shortly discuss these additional assumptions that are commonly employed. But first, we elucidate some key implications of Granger’s definition of causality.

#### 1.2 Properties of Granger Causality

##### 1.2.1 Deterministic Causation

It is impossible to find a cause for a series that is self-deterministic. Thus, if \( X_t \) is expressible as a deterministic function of its previous values, then no additional information can alter this “prediction”, and hence no other cause is necessary. In the light of Taken’s embedding theorem [13], this has an important implication. For certain classes of dynamical systems specified by systems of ordinary differential equations, a single variable may be able to perfectly reconstruct the dynamics through Taken’s delay-coordinate construction, implying that other variables may be found to be causally superfluous as far as Granger’s notion is concerned.

##### 1.2.2 Reflexivity, Symmetry, & Transitivity

Clearly, causality is not required to be symmetric; \( X_t \) may cause \( Y_t \) but not the other way around. Additionally, \( X_t, X_{t+1} \) could be independent for all \( t \neq t' \), and yet \( Y_t \) could be a cause for \( X_t \). Thus, \( X_t \) is not required to be a cause for itself, i.e., causality is not necessarily reflexive. It is also not required to be transitive (See Example 1 in [11]), i.e., \( X_t \) causes \( Y_t \) and \( Y_t \) causes \( Z_t \), does not necessarily imply \( X_t \) causes \( Z_t \) in the sense of Definition 2.

##### 1.2.3 Missing Variables & Unobserved Causes

Missing variables can induce spurious causality. Unobserved common causes are particularly important. For example [11], suppose:

\[
Z_t = a_t \quad (9)
\]

\[
X_t = a_{t-1} + b_t \quad (10)
\]

\[
Y_t = a_{t-2} + c_t \quad (11)
\]

where \( a_t, b_t, c_t \) are independent white noise processes. Here \( Z_t \) is a common cause. However, if we only observe \( X_t \) and \( Y_t \), then \( X_t \) seems to be causing \( Y_t \). There is no general fix for this; but it has been shown that such one-way spurious causation is unlikely in physical systems, and a two-way or feedback relationship is a more likely outcome with unobserved common causes [14].

##### 1.3 Additional Assumptions in Standard Approaches

Inferring causality in the mean (See Eq. (8)) is easier, and if one is satisfied with using minimum mean square prediction error as the criterion to evaluate incremental predictive power, then one may use linear one-step-ahead least squares predictors to obtain an operational procedure from Eq. (8): if \( \text{VAR}(X_t) \) is the variance of one-step forecast error of \( X_{n+1} \) given \( J_n \), then \( Y_t \) is a prima facie cause of \( X_t \) with respect to \( J_n \) if:

\[
\text{VAR}(X_t|J_n) < \text{VAR}(X_t|J_n)
\]  

(12)

Testing for bivariate Granger causality in the mean involves estimating a linear reduced-form vector autoregression:

\[
X_t = A(L)X_t + B(L)Y_t + U_{Xt}
\]  

(13)

\[
Y_t = C(L)X_t + D(L)Y_t + V_{Yt}
\]  

(14)

where \( A(L), B(L), C(L) \), and \( D(L) \) are one-sided lag polynomials in the lag operator \( L \) with roots all-distinct, and outside the unit circle. The regression errors \( U_{Xt}, V_{Yt} \) are assumed to be mutually independent and individually i.i.d. with zero mean and constant variance. A standard joint test (F or \( \chi^2 \)-test) is used to determine whether lagged \( Y \) has significant linear predictive power for current \( X \). The null hypothesis that \( Y \) does not strictly Granger cause \( X \) is rejected if the coefficients on the elements in \( B(L) \) are jointly significantly different from zero.

Linear tests pre-suppose restrictive and often unrealistic [15, 16] structure on data. Brock [17] presents a simple bivariate model to analytically demonstrate the limitations of linear tests in uncovering nonlinear influence. To address this issue, a number of nonlinear tests have been reported, e.g., with generalized autoregressive conditional heteroskedasticity (GARCH) models [18], using wavelet transforms [19], or heuristic additive relationships [20]. However,
these approaches often assume the class of allowed non-linearities; thus not quite alleviating the problem of pre-supposed structure. This is not just an academic issue: Granger causality has been shown to be significantly sensitive to non-linear transformations [21].

Non-parametric approaches, e.g. the Hiemstra-Jones (HJ) test [22], on the other hand, attempt to completely dispense with pre-suppositions on the causality structure. Given two series $X_t$ and $Y_t$, the HJ test (which is a modification of the Baek-Brock test [24]) uses correlation integrals to test if the probability of similar futures for $X_t$ given similar pasts, change significantly if we condition instead on similar pasts for both $X_t$ and $Y_t$ simultaneously. Nevertheless, the data series are required to be ergodic, stationary, and absolutely regular i.e. $\beta$-mixing, with an upper bound on the rate at which the $\beta$-coefficients approach zero [24], in order to achieve consistent estimation of the correlation integrals. The additional assumptions beyond ergodicity and stationarity serve to guarantee that sufficiently separated fragments of the data series are nearly independent. The HJ test and its variants [25], [26] have been quite successful in econometrics; uncovering nonlinear causal relations between money & income [24], aggregate stock returns & macroeconomic factors [27], currency future returns [28] and stock price & trading volume [22]. Surprisingly, despite clear evidence that linear tests typically have low power in uncovering nonlinear causation [23], [28], application of non-parametric tests has been limited in areas beyond financial, or macroeconomic interests.

2 Contribution Of The Present Work

The HJ test and its variants are specifically designed to detect Granger causality at a pre-specified significance level; there is no obvious extension by which a generative nonlinear model of this cross-dependence may be distilled from the data at hand. We are left with an oracle in a black box - it answers questions without any insight on the dynamical structure of the system under inquiry. On the other hand, linear regression-based, as well as parametric nonlinear approaches, have one discernible advantage; they produce generative models of causal influence between the observed variables. Hiemstra’s suggestion was to view non-parametric tests purely as a tool for uncovering existence of non-linearities in system dynamics; leaving the task of detailed investigation of dynamical structure to parametric model-based approaches:

- Hiemstra et al. [22]

Although the nonlinear (non-parametric) approach to causality testing presented here can detect nonlinear causal dependence with high power, it provides no guidance regarding the source of the nonlinear dependence. Such guidance must be left to theory, which may suggest specific parameterized structural models.

This is perhaps the motivation behind applying the HJ test in [22] to error residuals from an estimated linear autoregressive model; by removing linear structure using regression the authors conclude that any additional causal influence must be nonlinear in origin. However is it completely unreasonable to ask for a generative model of causal cross-dependence, where we are unwilling to a priori specify any dynamical structure? The central objective of the present work is to show that such an undertaking is indeed fruitful; beginning with sequential observations on two variables, we may infer non-heuristic generative models of causal influence with no presupposition on the nature of the hidden dynamics, linear or nonlinear. This however is a non-trivial exercise; if we are to allow for the appearance of dynamical models with unspecified and unrestricted structure, we need to rethink the framework within which such inference is carried out. It is well understood that this task is unattainable in the absence of at least some broad assumptions on the statistical nature of the sources [11], particularly on the nature of temporal or sequential variation in the underlying statistical parameters. We restrict ourselves to ergodic and stationary sources, and additionally assume that the data streams take values within finite sets; i.e., we only consider ergodic, stationary quantized stochastic processes (explicit definition given later).

We briefly recapitulate an earlier result that underlying generators for individual data streams from ergodic stationary quantized processes may be represented as probabilistic automata. And then we show that for two streams, generative models of causal influence may be represented as generalized probabilistic automata, referred to as crossed automata. Our task then reduces to inferring these crossed machines from data, in the absence of a priori knowledge of structure and parameters involved. True to the possible asymmetric nature of
causality, we show that such inferred logical machines are direction-specific; the crossed machine capturing the influence from stream $s_A$ to stream $s_B$ is not required to be identical to the one from $s_B$ to $s_A$. Additionally, we show that absence of causal influence between data streams manifests as a trivial crossed machine, and the existence of such trivial representations in both directions is necessary and sufficient for statistical independence between the data streams under consideration.

Our ability to find generative models of causal dependence allows us to carry out out-of-sample prediction. In contrast, the HJ test is vulnerable to Granger’s objection [11], that in absence of an inferred model, one is not strictly adhering to the original definition of Granger causality, which requires improved predictive ability, and not simply analysis of past data. Model-based approaches can indeed make and test predictions, but at the cost of the pre-imposed model structure (See proposed recipe in [11]). The current approach, in contrast, produces generative models without pre-supposed structure; and is therefore able to carry out and test predictions without the aforementioned cost.

In addition to obtaining explicit models of causal dependence between observed data streams, the present work identifies a new test for Granger causality, for quantized processes (i.e. processes which take values within a finite set). Our approach involves computing the coefficient for causal dependence $\gamma_{A,B}$, from the process generating a stream $s_A$ to the process generating a stream $s_B$. It is defined as the ratio of the expected change in the entropy of the next-symbol distribution in stream $s_B$ conditioned over observations in the stream $s_A$ to the entropy of the next-symbol distribution in stream $s_B$, conditioned on the fact that no observations are made on stream $s_A$. We show that $\gamma_{A,B}$ takes values on the closed unit interval, and higher values indicate stronger separation of $s_A$ from $s_B$, i.e., a higher degree of causal influence.

It is important to note that the state of the art techniques, including the HJ test, merely “test” for the existence of a causal relationship; setting up the problem in the framework of a classical binary hypothesis testing. No attempt is made to infer the degree of the causal connection, once the existence of such a relationship is statistically established. Perhaps one may point to the significance value at which the test is passed (or failed); but statistical significance of the tests is not, at least in any obvious manner, related to the degree of causality. In contrast, our definition of $\gamma_{A,B}$ has this notion clearly built in. As we stated earlier, higher values of the coefficient indicate a stronger causal connection; and $\gamma_{B,A} = 1$ indicates a situation in which the symbol in the immediate future of $s_B$ is deterministically fixed given the past values of $s_A$, but looks completely random if only the past values of $s_B$ are available.

While the HJ test and the computational inference of the coefficient of causality imposes similar assumptions on the data, the assumptions in the latter case are perhaps more physically transparent. Both approaches require ergodicity and stationarity; the HJ test further requires the processes to be absolutely regular ($\beta$-mixing), with a certain minimum asymptotic decay-rate of the $\beta$ coefficients (See [29], footnote on pg. 4, and [24]). Absolute regularity is one of the several ways one can have weak dependence; essentially implying that two sufficiently separated fragments of a data stream are nearly independent. Our algorithms also require weak dependence in addition to stationarity and ergodicity; however instead of invoking mixing coefficients, we require that the processes have a finite number of causal states (See Figure 2). Causal states are equivalence classes of histories that produce similar futures; and hence a finite number of causal states dictates that we need a finite number of classes of histories for future predictions.

As for the computational cost of the algorithms, we show that the inference of the crossed automata is PAC-efficient [10]; i.e., we can infer good models with high probability, in asymptotically polynomial time and sample complexity. The HJ test may well have good computational properties; but the literature lacks a detailed investigation.

In summary, the key contributions of the present work may be enumerated as:

1) A new non-parametric test for Granger causality for quantized processes is introduced. Going beyond binary hypothesis testing, we quantify the notion of the degree of causal influence between observed data streams, without pre-supposing any particular model structure.

2) Generative models of causal influence are shown to be inferable with no a priori imposed dynamical structure beyond ergodicity, stationarity, and a form of weak dependence. The explicit generative models may be used for prediction.

3) The proposed algorithms are shown to be PAC-efficient.

2.1 Organization

The rest of the paper is organized as follows: Section 3 makes precise the notion of quantized stochastic processes, and the connection to probabilistic automata. Some of the material in this section has appeared elsewhere [31], but is included for the sake of completeness, and due to some key technical differences, and extensions to the exposition. Section 4 presents the framework for representing generative models for cross-dependence; introducing crossed probabilistic automata. The coefficient of causal dependence is defined, and the directionality of the causality is investigated in this context. Section 5 presents algorithm $\text{GenESeSS}$ for inferring generative self-models from individual data streams. Again, $\text{GenESeSS}$ has been reported earlier in [31], but is included here for the sake of completeness. Section 6 presents algorithm $\text{xGenESeSS}$, which infers crossed automata from pairs of data streams, as generative models of direction-specific causal dependence. The complexity and PAC-efficiency of $\text{xGenESeSS}$ is investigated. Section 7 deals with the inference of causality networks between multiple data streams, and the fusion of future predictions from inferred crossed models. A simple application of the developed theory is illustrated in Section 8, where the causality network between weekly search-frequency data (data source: Google Trends) for a chosen list of keywords is computed. The paper is concluded in Section 9.

3 Quantized Stochastic Processes & Probabilistic Automata

Our approach hinges upon effectively using probabilistic automata to model stationary, ergodic processes. Our automata models are distinct to those reported in the literature [32], [33]. The details of this formalism can be found in [31]; we include a brief overview here for completeness.

Notation 1. $\Sigma$ is a finite alphabet of symbols. The set of all finite but possibly unbounded strings over $\Sigma$ is denoted by $\Sigma^*$. The set of finite strings over $\Sigma$ form a concatenative monoid, with the empty word $\lambda$ as identity. The set of strictly infinite strings on $\Sigma$ is denoted as $\Sigma^\omega$, where $\omega$ denotes the first transfinite cardinal. For a string $x$, $|x|$ denotes its length, and for a set $A$, $|A|$ denotes its cardinality. Also, $\Sigma^* = \{x \in \Sigma^* | |x| \leq d\}$. Defining a discrete time $\Sigma$-valued strictly stationary, ergodic stochastic process, $H$.

\begin{equation}
H = \{X_t : X_t \text{ is a } \Sigma \text{-valued random variable, } t \in \mathbb{N} \cup \{0\}\}
\end{equation}

A process is ergodic if moments may be calculated from a sufficiently long realization, and strictly stationary if moments are time-invariant.

We next formalize the connection of QSPs to PFSA generators. We develop the theory assuming multiple realizations of the QSP $H$. \(\ldots\)}
and fixed initial conditions. Using ergodicity, we will then able to apply our construction to a single sufficiently long realization, where initial conditions cease to matter.

**Definition 4** (σ-Algebra On Infinite Strings). For the set of infinite strings on Σ, we define ℬ to be the smallest σ-algebra generated by the family of sets \( \{ X^n : x \in \Sigma^* \} \).

**Lemma 1.** Every QSP induces a probability space \((\Sigma^\omega, \mathcal{B}, \mu)\).

**Proof:** Assuming stationarity, we can construct a probability measure \( \mu : \mathcal{B} \to [0,1] \) by defining for any sequence \( x \in \Sigma^* \setminus \{ \lambda \} \), and a sufficiently large number of realizations \( N_0 \) (assuming ergodicity):

\[
\mu(x^{\omega}) = \lim_{N_0 \to \infty} \frac{\# \text{ of initial occurrences of } x}{\# \text{ of initial occurrences of all sequences of length } |x|}
\]

and extending the measure to elements of \( \mathcal{B} \) via at most countable sums. Thus \( \mu(x^{\omega}) = \sum x \in \Sigma \mu(x^{\omega}) = 1 \), and for the null word \( \mu(\lambda^{\omega}) = \mu(1^{\omega}) = 1 \).

**Notation 2.** For notational brevity, we denote \( \mu(x^{\omega}) = Pr(x) \).

Classically, automaton states are equivalence classes for the Nerode relation; two strings are equivalent if and only if any finite extension of the strings is either both in the language under consideration, or neither are [12]. We use a probabilistic extension [13].

**Definition 5** (Probabilistic Nerode Equivalence Relation). \((\Sigma^\omega, \mathcal{B}, \mu)\) induces an equivalence relation \( \sim_N \) on the set of finite strings \( \Sigma^* \) as:

\[
\forall x, y \in \Sigma^*, x \sim_N y \iff \exists z \in \Sigma^* \left( Pr(xz) = Pr(yz) = 0 \right)
\]

(16)

**Notation 3.** For \( x \in \Sigma^* \), the equivalence class of \( x \) is \([x]\).

It is easy to see that \( \sim_N \) is right invariant, i.e.

\[
x \sim_N y \Rightarrow xz \sim_N yz
\]

(17)

A right-invariant equivalence on \( \Sigma^* \) always induces an automaton structure; and hence the probabilistic Nerode relation induces a probabilistic automaton: states are equivalence classes of \( \sim_N \), and the transition structure arises as follows: For states \( q_i, q_j \), and \( x \in \Sigma^* \),

\[
([x] = q) \land ([xr] = q') \Rightarrow q \xrightarrow{r} q'
\]

(18)

Before formalizing the above construction, we introduce the notion of probabilistic automata with initial, but no final, states.

**Definition 6** (Initial-Marked PFSA). An initial marked probabilistic finite state automaton (an Initial-Marked PFSA) is a quintuple \((Q, \Sigma, \delta, \pi, q_0)\), where \( Q \) is a finite state set, \( \Sigma \) is the alphabet, \( \delta : Q \times \Sigma \to Q \) is the state transition function, \( \pi : Q \times \Sigma \to [0,1] \) specifies the conditional symbol-generation probabilities, and \( q_0 \in Q \) is the initial state, and \( \pi \) are recursively extended to arbitrary \( y = \sigma x \in \Sigma^* \) as follows:

\[
\forall q \in Q, \delta(q, \lambda) = q
\]

(19a)

\[
\delta(q, \sigma x) = \delta(\delta(q, \sigma), x)
\]

(19b)

\[
\forall q \in Q, \pi(q, \lambda) = 1
\]

(19c)

\[
\pi(q, \sigma x) = \pi(q, \sigma) \pi(\delta(q, \sigma), x)
\]

(19d)

Additionally, we impose that for distinct states \( q_i, q_j \in Q \), there exists a string \( x \in \Sigma^* \), such that \( \delta(q_i, x) = q_j \), and \( \pi(q_i, x) > 0 \).

Note that the probability of the null word is unity from each state. If the current state and the next symbol is specified, our next state is fixed; similar to Probabilistic Deterministic Automata [35]. However, unlike the latter, we lack final states in the model. Additionally, we assume our graphs to be strongly connected. Later we will remove initial state dependence using ergodicity. Next we formalize how a PFSA arises from a QSP.

**Lemma 2** (PFSA Generator). *Every Initial-Marked PFSA \( G = (Q, \Sigma, \pi, q_0) \) induces a unique probability measure \( \mu_G \) on the measurable space \((\Sigma^\omega, \mathcal{B})\).*

**Proof:** Define set function \( \mu_G \) on the measurable space \((\Sigma^\omega, \mathcal{B})\):

\[
\mu_G(\emptyset) = 0
\]

(20a)

\[
\forall x \in \Sigma^*, \mu_G(x^{\omega}) = \pi(q_0, x)
\]

(20b)

\[
\forall x, y \in \Sigma^*, \mu_G((x,y)^{\omega}) = \pi_0(x^{\omega}) + \pi_0(y^{\omega})
\]

(20c)

Countable additivity of \( \mu_G \) is immediate, and we have (See Definition 6):

\[
\mu_G(\Sigma^\omega) = \mu_G(\lambda^{\omega}) = \pi(q_0, \lambda) = 1
\]

(21)

implying that \((\Sigma^\omega, \mathcal{B}, \mu_G)\) is a probability space.

We refer to \((\Sigma^\omega, \mathcal{B}, \mu_G)\) as the probability space generated by the Initial-Marked PFSA \( G \).

**Lemma 3** (Probability Space To PFSA). If the probabilistic Nerode relation corresponding to a probability space \((\Sigma^\omega, \mathcal{B}, \mu)\) has a finite index, then the latter has an initial-marked PFSA generator.

**Proof:** Let \( Q \) be the set of equivalence classes of the probabilistic Nerode relation (Definition 5), and define functions \( \delta : Q \times \Sigma \to Q \), \( \pi : Q \times \Sigma \to [0,1] \) as:

\[
\delta([x], \sigma) = [x]\sigma
\]

(22a)

\[
\pi([x], \sigma) = \frac{Pr(x\sigma)}{Pr(x)}
\]

(22b)

where we extend \( \delta, \pi \) recursively to \( y = \sigma x \in \Sigma^* \) as

\[
\delta(q, \sigma x) = \delta(\delta(q, \sigma), x)
\]

(23a)

\[
\pi(q, \sigma x) = \pi(q, \sigma) \pi(\delta(q, \sigma), x)
\]

(23b)

For verifying the null-word probability, choose a \( x \in \Sigma^* \) such that \([x] = q\) for some \( q \in Q \). Then, from Eq. (25b), we have:

\[
\pi(q, \lambda) = \frac{Pr(x\lambda)}{Pr(x)}
\]

for any \( x' \in \Sigma^* \) \( \Rightarrow \pi(q, \lambda) = 1 \)

(24)

Finite index of \( \sim_N \) implies \( |Q| < \infty \), and hence denoting \([1]\) as \( q_0 \), we conclude: \( G = (Q, \Sigma, \pi, q_0) \) is an Initial-Marked PFSA. Lemma 2 implies that \( G \) generates \((\Sigma^\omega, \mathcal{B}, \mu)\), which completes the proof.

The above construction yields a minimal realization for the Initial-Marked PFSA, unique up to state renaming.

**Lemma 4** (QSP to PFSA). Any QSP with a finite index Nerode equivalence is generated by an Initial-Marked PFSA.

**Proof:** Follows immediately from Lemma 1(QSP to Probability Space) and Lemma 3(Probability Space to PFSA generator).

3.1 Canonical Representations

We have defined a QSP as both ergodic and stationary, whereas the Initial-Marked PFSA has a designated initial state. Next we introduce canonical representations to remove initial-state dependence. We use \( \Pi \) to denote the matrix representation of \( \pi \), i.e., \( \Pi_{ij} = \pi(q_i, \sigma_j) \), \( q_i \in Q, \sigma_j \in \Sigma \). We need the notion of transformation matrices \( \Gamma_{\sigma} \).

**Definition 7** (Transformation Matrices). For an initial-marked PFSA \( G = (Q, \Sigma, \delta, \pi, q_0) \), the symbol-specific transformation matrices \( \Gamma_{\sigma} \) \in \([0,1]^{Q \times Q}\) are:

\[
\Gamma_{\sigma}[ij] = \begin{cases} 
\pi(q_i, \sigma), & \text{if } \delta(q_i, \sigma) = q_j \\
0, & \text{otherwise}
\end{cases}
\]

(25)

Transformation matrices have a single non-zero entry per row, reflecting our generation rule that given a state and a generated symbol, the next state is fixed.

First, we note that, given an initial-marked PFSA \( G \), we can associate a probability distribution \( \varphi_{q} \) over the states of \( G \) for each \( x \in \Sigma^* \) in the following sense: if \( x = \sigma_1 \cdots \sigma_m \in \Sigma^* \), then we have:

\[
\varphi_{x} = \varphi_{\sigma_1} \cdots \varphi_{\sigma_m} = \frac{1}{|\Pi|} \prod_{j=1}^{m} \Gamma_{\sigma_j}
\]

(26)
where $\phi_i$ is the stationary distribution over the states of $G$. Note that there may exist more than one string that leads to a distribution $\phi_i$, beginning from the stationary distribution $\phi_i$. Thus, $\phi_i$ corresponds to an equivalence class of strings, i.e., $x$ is not unique.

**Definition 8 (Canonical Representation).** An initial-marked PFSA $G = (Q, \Sigma, \delta, \pi, q_0)$ uniquely induces a canonical representation $(Q', \Sigma, \delta', \pi')$, where $Q'$ is a subset of the set of probability distributions over $Q$, and $\delta': Q' \times \Sigma \rightarrow Q'$, $\pi': Q' \times \Sigma \rightarrow [0, 1]$ are constructed as follows:

1. Construct the stationary distribution on $Q$ using the transition probabilities of the Markov chain induced by $G$, and include this as the first element $\phi_1$ of $Q'$. Note that the transition matrix for $G$ is the row-stochastic matrix $M \in [0, 1]^{Q \times [Q]}$, with $M_{ij} = \sum_{q \in Q} \phi_i(q, \sigma) \pi(q, \sigma)$, and hence $\phi_1$ satisfies:
   \[
   \phi_1 M = \phi_1
   \]  
   (27)

2. Define $\delta'$ and $\pi'$ recursively:
   \[
   \delta'(\phi_i, \sigma) = \frac{1}{\|\phi_i\|_1} \phi_i \Gamma_{i\sigma} \triangleq \phi_{i\sigma}
   \]  
   (28)
   \[
   \pi'(\phi_i, \sigma) = \phi_i \Pi
   \]  
   (29)

For a QSP $H$, the canonical representation is denoted as $C_H$.

**Lemma 5 (Properties of Canonical Representation).** Given an initial-marked PFSA $G = (Q, \Sigma, \delta, \pi, q_0)$:

1. The canonical representation is independent of the initial state.
2. The canonical representation $(Q', \Sigma, \delta', \pi')$ contains a copy of $G$ in the sense that there exists a set of states $Q' \subseteq Q'$ such that there exists a one-to-one map $\zeta: Q \rightarrow Q'$, with:
   \[
   \forall q \in Q, \forall \sigma \in \Sigma \left\{ \pi'(\zeta(q), \sigma) = \pi'((q), \sigma) \right\} \]  
   (30)

3. If during the construction (beginning with $\phi_1$) we encounter $\phi_2 = \zeta(q)$ for some $x \in \Sigma^*$, $q \in Q$ and any map $\zeta$ as defined in (2), then we stay within the graph of the copy of the initial-marked PFSA for all right extensions of $x$.

**Proof:** (1) follows the ergodicity of QSPs, which makes $\phi_1$ independent of the initial state in the initial-marked PFSA.

2. The canonical representation subsumes the initial-marked representation in the sense that the states of the latter may themselves be seen as degenerate distributions over $Q$, i.e., by letting:
   \[
   E = \{ e' | e \in [0, 1]^{Q}, i = 1, \ldots, |Q| \}\]  
   (31)

   denote the set of distributions satisfying:
   \[
   e'_{ij} = \begin{cases} 
   1, & \text{if } i = j \\
   0, & \text{otherwise}
   \end{cases}
   \]  
   (32)

3. (3) follows from the strong connectivity of $G$. □

**Lemma 3** implies that initial states are unimportant; we may denote the initial-marked PFSA induced by a QSP $H$, with the initial marking removed, as $P_{\mu}$, and refer to it simply as a "PFSA." States in $P_{\mu}$ are representable as states in $C_H$ as elements of $E$. Note that we always encounter a state arbitrarily close to some element in $E$ in the canonical construction starting from the stationary distribution $\phi_1$ on the states of $P_{\mu}$. However, before we go further, we establish the existence of unique minimal realizations. Note that even if initial-marked PFSA are strongly connected, the canonical representations might not be.

**Definition 9 (Structural Isomorphism Between PFSA).** PFSA $G = (Q, \Sigma, \delta, \pi, q_0)$ and $G' = (Q', \Sigma, \delta', \pi')$, defined on the same alphabet $\Sigma$, are structurally isomorphic if there exists a bijective mapping $\xi: Q \rightarrow Q'$ such that:
   \[
   \forall q \in Q, \forall \sigma \in \Sigma \left\{ \xi(\delta(q, \sigma)) = \delta'(\xi(q), \sigma), \pi'(\xi(q), \sigma) = \pi'(\xi(q), \sigma) \right\} \]  
   (33)

Note, bijectivity of $\xi$ requires $|Q| = |Q'|$. Structural isomorphism between two PFSA implies that there exists a permutation of the states such that one is transformed to the other. Thus, structurally isomorphic PFSA encode the same QSP.

**Theorem 1 (Existence Of Unique Strongly Connected Minimal Realization).** If the probabilistic Nerode relation corresponding to a probability space $(\Sigma^*, B, \mu)$, representing a stationary ergodic QSP, has a finite index, then it has a strongly connected PFSA generator unique up to structural isomorphism.

**Proof:** First we use the construction described in Lemma 3 to obtain a PFSA generator $G = (Q, \Sigma, \delta, \pi, q_0)$ for the finite index Nerode relation $\sim_N$ corresponding to a probability space $(\Sigma^*, B, \mu)$. Note that since the QSP that the probability space represents is ergodic, we can drop the initial state from the construction of Lemma 3.

Let $G' = (Q', \Sigma, \delta'_N, \pi'_N)$ be a strongly connected component of $G$, i.e., we have $Q' \subseteq Q$, and $\delta'_N, \pi'_N$ are the restriction of the corresponding functions to the possibly smaller set of states, and $(Q', \delta'_N)$ defines a strongly connected graph with $Q'$ as the set of nodes, and there is a labeled edge $q_i \rightarrow q_j$ if $\delta'_N(q_i, \sigma) = q_j$.

Let $q_0 \in Q'$, such that $3x_0 \in \Sigma^*$, $[x_0] = q_0$, such that $\mu(x_0 \Sigma^*) > 0$.

Let $H$ be an initial marked PFSA obtained by augmenting $G'$ with $q_0$ as the initial state, i.e., $H = (Q', \Sigma, \delta'_N, \pi'_N, q_0)$. Let us denote:
   \[
   E_H = \{ [x_0] : x \in \Sigma^* \}
   \]  
   (34)

Let $E$ be the set of equivalence classes of $\sim_N$. It is immediate that:
   \[
   E_H \subseteq E
   \]  
   (35)

Also, since $H$ is strongly connected, and any right extension of $x_0$ terminates on some state $q' \in Q'$, it is immediate that there exists bijective map $H: Q' \rightarrow E_H$.

Let if possible there exist $E \in E$ such that $E \notin E_H$. And let $z \in \Sigma^*$, such that $z \in E$. Then, it follows that:
   \[
   \forall x' \in \Sigma^*, x_0 x' \sim_N z
   \]  
   (36)

which contradicts our assumption that the QSP is ergodic. Hence, we conclude that $E = E_H$, i.e., $H$ is a generator for $\sim_N$.

We claim that the map $H: Q' \rightarrow E$ is injective. To see this, assume if possible that for some distinct $q_1, q_2 \in Q'$:
   \[
   H(q_1) = H(q_2) = E \in E
   \]  
   (37)

Since $q_1, q_2$ are distinct, there exist strings $x_1, x_2 \in \Sigma^*$ such that $[x_1] \neq [x_2]$, which contradicts Eq. (37). Hence, we conclude that $H$ is a minimal realization. Since $G'$ is an arbitrary strongly connected component of $G$, and the above argument is valid for any permutation of the state labels, we conclude that $H$ is unique up to structural equivalence. This completes the proof.

To summarize, every PFSA $G = (Q, \Sigma, \delta, \pi, q_0)$ represents a probability space $(\Sigma^*, B, \mu)$ for any fixed initial state, and there is always a minimal realization that encodes the latter; however $G'$ could possibly be a non-minimal realization of the underlying probability space. Thus, given a PFSA $G = (Q, \Sigma, \delta, \pi, q_0)$, and a choice of an initial state $q_0$, we have two associated equivalence relations on $\Sigma^*$:

1. The transition equivalence $\sim_T$ defined by the graph of the PFSA, i.e. its transition structure and its states:
   \[
   x \sim_T y \text{ if } \delta(q_0, x) = \delta(q_0, y)
   \]  
   (38)

2. The probabilistic Nerode equivalence $\sim_N$ given by:
   \[
   x \sim_N y \text{ if } \forall z \in \Sigma^*, \delta(xz \Sigma^*) = \delta(yz \Sigma^*)
   \]  
   (39)

We have the following immediate result:

**Lemma 6 (Transition Equivalence).** Given a PFSA $G = (Q, \Sigma, \delta, \pi, q_0)$, and a choice of an initial state $q_0 \in Q$, the transition equivalence is necessarily a refinement of the corresponding Nerode equivalence. The two equivalences are identical if $G$ is a minimal realization.

**Proof:** Follows immediately by noting that:
   \[
   x \sim_N y \Rightarrow \delta(q_0, x) = \delta(q_0, y) \Rightarrow \forall z \in \Sigma^*, \delta(q_0, xz) = \delta(q_0, yz) \Rightarrow \forall z \in \Sigma^*, \mu(xz \Sigma^*) = \mu(yz \Sigma^*)
   \]  
   (40)

Next we introduce the notion of $\epsilon$-synchronization of probabilistic automata (See Figure 3). Synchronization of automata is fixing or
determining the current state; thus it is analogous to contexts in Rissanen’s “context algorithm” \[56]. We show that while not all PFSAs are synchronizable, all are \(\varepsilon\)-synchronizable.

**Theorem 2** (\(\varepsilon\)-Synchronization of Probabilistic Automata). For any QSP \(\mathcal{H}\) over \(\Sigma\), the PFSA \(\mathcal{P}_H\) satisfies:

\[
\forall \epsilon > 0, \exists \pi \in \Sigma^*, \exists \theta \in \mathbb{E}, ||\pi_x - \theta||_\infty \leq \epsilon \tag{41}
\]

**Proof:** We show that all PFSAs are at least approximately synchronizable \[37], \[38], which is not true for deterministic automata. If the graph of \(\mathcal{P}_H\) (i.e., the deterministic automaton obtained by removing the arc probabilities) is synchronizable, then Eq. (41) trivially holds true for \(\epsilon = 0\) for any synchronizing string \(x\). Thus, we assume the graph of \(\mathcal{P}_H\) to be non-synchronizable. From definition of non-synchronizability, it follows:

\[
\forall q_i, q_j \in \mathcal{Q}, \text{ with } q_i \neq q_j, \forall x \in \Sigma^*, \delta(q_i, x) \neq \delta(q_j, x) \tag{42}
\]

If the PFSA has a single state, then every string satisfies the condition in Eq. (41). Hence, we assume that the PFSA has more than one state. Now if we have:

\[
\exists x \in \Sigma^*, \frac{Pr(x)}{Pr(x')}, \text{where } x' = q_i, x = q_j \tag{43}
\]

then, by the Definition 5, we have a contradiction \(q_i = q_j\). Hence \(\exists \pi_0\) such that:

\[
\forall x \in \Sigma^*, \frac{Pr(x)}{Pr(x')}, \text{ where } x = q_i, x' = q_j \tag{44}
\]

Since:

\[
\sum_{x \in \Sigma} \frac{Pr(x)}{Pr(x')} = 1, \text{for any } x \text{ where } x = q_i
\]

we conclude without loss of generality \(\forall q_i, q_j \in \mathcal{Q}, \text{ with } q_i \neq q_j; \exists x \in \Sigma^*, \text{ where } x = q_i, x' = q_j \tag{45}
\]

It follows from induction that if we start with a distribution \(\pi\) on \(Q\) such that \(\pi = \pi_j = 0.5\), then for any \(\epsilon > 0\) we can construct a finite string \(x_i^{\epsilon}\) such that if \(\delta(q_i, x_i^{\epsilon}) = \delta(q_j, x_i^{\epsilon}) = q_i\), then the new distribution \(\pi'\) after executing \(x_i^{\epsilon}\) will satisfy \(\pi_j > 1 - \epsilon\). Recalling that \(\mathcal{P}_H\) is strongly connected, we note that, for any \(q_i \in \mathcal{Q}\), there exists a string \(y \in \Sigma^*\), such that \(\delta(q_i, y) = q_i\). Setting \(x_i^{\epsilon} = y\), we can ensure that the distribution \(\pi'\) obtained after execution of \(x_i^{\epsilon}\) satisfies \(\pi' > 1 - \epsilon\) for any \(\epsilon\) of our choice. For arbitrary initial distributions \(\pi\) on \(Q\), we must consider contributions arising from simultaneously executing \(x_i^{\epsilon}\) from states other than just \(q_i\) and \(q_j\). Nevertheless, it is easy to see that executing \(x_i^{\epsilon}\) implies that in the new distribution \(\pi'\), we have \(\pi_j' > \pi_i' + \epsilon\). It follows that executing the string \(x_1^{\epsilon}, x_2^{\epsilon}, \ldots, x_{j-1}^{\epsilon}, y, x_{j+1}^{\epsilon}, \ldots, x_{i-1}^{\epsilon}\), where

\[
n = \begin{cases} |Q| & \text{if } |Q| \text{ is even} \\ |Q| - 1 & \text{otherwise} \end{cases} \tag{46}
\]

would result in a final distribution \(\pi''\) which satisfies \(\pi''_{q_j} > 1 - \frac{1}{2} \epsilon\). Appropriate scaling of \(\epsilon\) then completes the proof. 

**Definition 10** (\(\varepsilon\)-synchronizing Strings). A string \(x \in \Sigma^*\) is \(\varepsilon\)-

synchronizing for a PFSA if:

\[
\exists \theta \in \mathbb{E}, ||\pi_x - \theta||_\infty \leq \epsilon \tag{47}
\]

Theorem 2 is an existential result, and does not yield an algorithm for computing synchronizing strings (See Theorem 4). We may estimate an asymptotic upper bound on such a search.

**Corollary 1** (To Theorem 2). At most \(O(1/\epsilon)\) strings from the lexicographically ordered set of all strings over the given alphabet need to be analyzed to find an \(\varepsilon\)-synchronizing string.

**Proof:** Theorem 2 multiplies entries from the \(\Pi\) matrix, which cannot be all identical (otherwise the states would collapse). Let the minimum difference between two unequal entries be \(\eta\). Then, following the construction in Theorem 2, the length \(\ell\) of the synchronizing string, up to linear scaling, satisfies: \(\eta = O(\epsilon), \text{ implying } \ell = O(\log(1/\epsilon)). \) Hence, the number of strings to be analyzed is at most all strings of length \(\ell\), where \(|\Sigma'| = |\Sigma|^{O(\log(1/\epsilon))} = O(1/\epsilon)\). 

### 3.2 Symbolic Derivatives

Computation of \(\varepsilon\)-synchronizing strings requires the notion of symbolic derivatives. PFSAs are not observable; we observe symbols generated from hidden states. A symbolic derivative at a given string specifies the distribution of the next symbol over the alphabet.

**Notation 4.** We denote the set of probability distributions over a finite set of cardinality \(k\) as \(\mathcal{D}(k)\).

**Definition 11** (Symbolic Count Function). For a string \(s\) over \(\Sigma\), the count function \(\# : \Sigma^* \rightarrow \mathbb{N} \cup \{0\}\), counts the number of times a particular substring occurs in \(s\). The count is overlapping, i.e., in a string \(s = 0001\), we count the number of occurrences of 00s as 0001 and 0001, implying \#00 = 2.

**Definition 12** (Symbolic Derivative). For a string \(s\) generated by a QSP over \(\Sigma\), the symbolic derivative \(\phi'(s) : \Sigma^* \rightarrow \mathcal{D}(|\Sigma| - 1)\) is defined:

\[
\phi'(s) = \sum_{\sigma \in \Sigma} \#(s \sigma) \Phi(s \sigma) \tag{48}
\]

Thus, \(\forall x \in \Sigma^*, \phi'(x)\) is a probability distribution over \(\Sigma\). \(\phi'(x)\) is referred to as the symbolic derivative at \(x\).

Note that \(\forall q_i \in \mathcal{Q}, \pi_i\) induces a probability distribution over \(\Sigma\) as \(\pi(q_i, r_1), \ldots, \pi(q_i, r_{|\Sigma|})\). We denote this as \(\pi_i(q_i)\).

We next show that the symbolic derivative at \(x\) can be used to estimate this distribution for \(q_i = |x|\), provided \(x\) is \(\varepsilon\)-synchronizing.

**Theorem 3** (\(\varepsilon\)-Convergence). If \(x \in \Sigma^*\) is \(\varepsilon\)-synchronizing, then:

\[
\forall \epsilon > 0, \lim_{|s| \rightarrow \infty} ||\phi(x) - \pi(x)||_\infty \leq \epsilon \tag{49}
\]

**Proof:** We use the Glivenko-Cantelli theorem \[59] on uniform convergence of empirical distributions. Since \(x\) is \(\varepsilon\)-synchronizing:

\[
\forall \epsilon > 0, \exists \theta \in \mathcal{E}, ||\pi_x - \theta||_\infty \leq \epsilon \tag{50}
\]

Recall that \(\mathcal{E} = \{|e| \in [0, 1], i = 1, \ldots, |\Omega|\}\) denotes the set of distributions over \(\mathcal{Q}\) satisfying:

\[
\epsilon(i) = \begin{cases} 1, & \text{if } i = j \\ 0, & \text{otherwise} \end{cases} \tag{51}
\]

Let \(x \in \varepsilon\)-synchronizing \(q \in \mathcal{Q}\). Thus, when we encounter \(x\) while reading \(s\), we are guaranteed to be distributed over \(\mathcal{Q}\) as \(\varphi\), where:

\[
||\pi_x - \theta||_\infty \leq \epsilon \Rightarrow \varphi = \alpha \varphi + (1 - \alpha)u \tag{52}
\]

where \(\alpha \in \{0, 1\}, \alpha \geq 1 - \epsilon, \text{ and } u\) is an unknown distribution over \(\mathcal{Q}\). Defining \(A_\alpha = \alpha \pi(q_i) + (1 - \alpha)\Sigma_{j=1}^{|\mathcal{Q}|} u(q_j)\), we note that \(\phi'(x)\) is an empirical distribution for \(A_\alpha\), implying:

\[
\lim_{|s| \rightarrow \infty} \|\phi(x) - \pi(q_i)\|_\infty = \lim_{|s| \rightarrow \infty} \|\phi(x) - A_\alpha - A_\alpha - \pi(q_i)\|_\infty \\
= a.s. 0 \text{ by Glivenko-Cantelli}
\]

\[
\leq \lim_{|s| \rightarrow \infty} \|\phi(x) - A_\alpha\|_\infty + \lim_{|s| \rightarrow \infty} \|A_\alpha - \pi(q_i)\|_\infty \\
\leq a.s. (1 - \alpha) \|\pi(q_i) - \pi(q_i)\|_\infty \leq a.s. \epsilon
\]
This completes the proof.

**Corollary 2** (To Theorem 3 Right Extension of $\varepsilon$-Synchronizing Strings). If $x \in \Sigma^*$ is $\varepsilon$-synchronizing, then $\exists \tau \in \Sigma$, such that $x\tau \in \varepsilon'$-synchronizing with $\varepsilon' = \mathcal{C}_\varepsilon$, and $C_\varepsilon$ is the finite constant:

$$C_\varepsilon = \max_{q_i, q_j \in \mathcal{Q}, \varepsilon > 0} \frac{\mathcal{P}(q_i, \varepsilon)}{\mathcal{P}(q_j, \varepsilon)} < \infty$$

**Proof:** Let $x \in \Sigma^*$ be $\varepsilon$-synchronizing. Definition 10 implies that:

$$\exists \sigma \in \Sigma^* \text{ s.t. } \mathcal{H}_1(\varepsilon, |x| - \theta, \varepsilon) \leq \varepsilon$$

We note that if the Nerode relation has a single equivalence class (i.e., the underlying minimal PFSA has a single state), then the result holds true for every $\sigma \in \Sigma$. Hence, we assume that the minimal realization of the underlying PFSA has more than one state.

Without loss of generality, let $\theta(1) = 1$, implying (Definition 10):

$$\mathcal{P}(_1) > 1 - \varepsilon$$

Since we assume the underlying PFSAs to be strongly connected, there exists $\nu^* \in \Sigma^*$ such that $\mathcal{P}(q_i, \nu^*) \neq q_j^*$, and $\mathcal{P}(q_i, \nu^*) > 0$. We compute $\mathcal{P}_{\nu^*}$ explicitly, using Eq. (26), and note that if $\mathcal{P}(q_i, \nu^*) = q_j^* \neq q_i^*$, then we have:

$$\mathcal{P}_{\nu^*} = \mathcal{P}(q_i, \nu^*) | 1 - \varepsilon$$

(56)

where $\forall \varepsilon, \varepsilon_0 \geq 0, \sum_{\varepsilon_0 | \varepsilon^*} \mathcal{P}(q_i, \varepsilon^*) = \sum_{\varepsilon_0 | \varepsilon^*} \mathcal{P}(q_i, \varepsilon^*) \varepsilon_0$

$$\Rightarrow \mathcal{P}_{\nu^*} = \frac{1}{1 + C} \mathcal{P}(q_i, \varepsilon^*)$$

(57)

where $C = \max_{\varepsilon_0 | \varepsilon^*} \mathcal{P}(q_i, \varepsilon^*) < \infty$

$$\Rightarrow e' = \frac{1}{1 + C} \leq \mathcal{C} \leq \mathcal{C}_0$$

(58)

This completes the proof.

**Remark 1** ($C_0$ As A System Property). It is crucial to note that the above argument remains valid for any right extension of an $\varepsilon$-synchronizing string, as long as the probability of that extension being generated from the synchronized state is non-zero. Specifically, note that the argument in Corollary 2 is valid for any $\nu^*$ as long as the probability of generating $\nu^*$ from state $q_i$ is non-zero (to ensure finiteness of $c$). Also, note that $C_0$ is a property of the underlying PFSA, and is independent of $x$. This would be important in establishing the efficient PAC-learnability of QSPs with finite number of causal states using PFSA as the hypothesis class.

### 3.3 Computation of $\varepsilon$-synchronizing Strings

Next we describe identification of $\varepsilon$-synchronizing strings given a sufficiently long observed string (i.e. a sample path) $x$. Theorem 2 guarantees existence, and Corollary 1 establishes that $O(1/\varepsilon)$ substrings need to be analyzed till we encounter an $\varepsilon$-synchronizing string. These do not provide an executable algorithm, which arises from an inspection of the geometric structure of the set of probability vectors over $\Sigma$, obtained by constructing $\phi(x)$ for different choices of the candidate string $x$.

**Definition 13** (Derivative Heap). Given a string $x$ generated by a QSP, a derivative heap $D' : \Sigma^* \rightarrow P(\Sigma^*)$ is the set of probability distributions over $\Sigma$ calculated for a subset of strings $L \subset \Sigma^*$ as:

$$D'(L) = \{\phi(x) : x \in L \subset \Sigma^*\}$$

(59)

**Lemma 7** (Limiting Geometry). Let us define:

$$D_\infty = \lim_{L \rightarrow \infty} D'(L)$$

(60)

If $\mathcal{H}_\infty$ is the convex hull of $D_\infty$, and $u$ is a vertex of $\mathcal{H}_\infty$, then $u \in Q$, such that $u = \mathcal{P}(q_i, \cdot)$

(61)

**Proof:** Recalling Theorem 2 the result follows from noting that any element of $D_\infty$ is a convex combination of elements from the set $[\mathcal{P}(q_i, \cdot), \cdots, \mathcal{P}(q_{|q|}, \cdot)]$.

**Lemma 7** does not claim that the number of vertices of the convex hull of $D_\infty$ equals the number of states, but that every vertex corresponds to a state. We cannot generate $D_\infty$ since we have a finite observed string $x$, and we can calculate $\phi(x)$ for a finite number of $x$. Instead, we show that choosing a string corresponding to the vertex of the convex hull of the heap, constructed by considering $O(1/\varepsilon)$ strings, gives us an $\varepsilon$-synchronizing string with high probability.

**Theorem 4** (Derivative Heap Approx.). For $s$ generated by a QSP, let $D'(L)$ be computed with $L = \Sigma^{\theta \log(1/\varepsilon)}$. If $x_0 \in \Sigma^{\theta \log(1/\varepsilon)}$, $\phi(x_0)$ is a vertex of the convex hull of $D'(L)$, then

$$Pr(x_0 \text{ is not } \varepsilon\text{-synchronizing}) < \varepsilon^{1/4}$$

(62)

where $p_0$ is the probability of encountering $x_0$ in $s$.

**Proof:** The result follows from Sanov’s Theorem 20 for convex set of probability distributions. If $|s| \rightarrow \infty$, then $x_0$ is guaranteed to be $\varepsilon$-synchronizing (Theorem 2 and Corollary 1). Denoting the number of times we encounter $x_0$ in $s$ as $n(s)$, and since $D_\infty$ is a convex set of distributions (allowing us to drop the polynomial factor in Sanov’s bound), we apply Sanov’s Theorem to the case of finite $s$:

$$Pr(k \leq \text{KL}^+(\phi(x_0) || \phi_s) \leq \varepsilon^{1/4})$$

(63)

where $\text{KL}(||)$ is the Kullback-Leibler divergence. Using Lemma 2:

$$\frac{1}{4} \|\phi(x_0) - \phi_s||_\infty^2 \leq \text{KL}(\phi(x_0) || \phi_s)$$

(64)

and $n(s) \rightarrow n(s)_0$, where $p_0 > 0$ is the stationary probability of encountering $x_0$ in $s$, we conclude:

$$Pr\left(\frac{1}{4} \|\phi(x) - \phi_s||_\infty \leq \varepsilon\right) \leq e^{-\varepsilon^{1/4}}$$

(65)

$$Pr\left(\|\phi(x) - \phi_s||_\infty \leq 4\varepsilon\right) \leq e^{-\varepsilon^{1/4}}$$

(66)

$$Pr\left(\|\phi(x) - \phi_s||_\infty \leq \varepsilon\right) \leq e^{-\varepsilon^{1/4}}$$

(67)

which completes the proof.

### 4 Probabilistic Models For Cross-talk

Consider two ergodic stationary QSPs $\mathcal{H}_A, \mathcal{H}_B$ evolving over two finite alphabets $\Sigma_A, \Sigma_B$ respectively. We make no additional assumptions as to the properties of the two alphabets, other than requiring that they be finite, i.e., $\Sigma_A, \Sigma_B$ may be identical, disjoint or have different cardinalities.

The dynamical dependence of the process $\mathcal{H}_B$ on the first process $\mathcal{H}_A$ is assumed to be dictated by the cross-talk map $F$ (defined next), which specifies the probability with which a string might transpire in the second process, given some specific string in the first.

**Notation 5.** Given a finite alphabet $\Sigma$ and the corresponding set of strictly infinite strings $\Sigma^\omega$, and the $\sigma$-algebra $\mathcal{B}$ as constructed in Definition 2, we denote the set of all probability spaces of the form $(\Sigma^\omega, \mathcal{B}, \mu)$ as $\mathcal{P}_\mathcal{B}$.

**Definition 14** (Cross-talk Map $F$). Given stationary ergodic QSPs $\mathcal{H}_A, \mathcal{H}_B$ over finite alphabets $\Sigma_A, \Sigma_B$ respectively, the dependency of $\mathcal{H}_B$ on $\mathcal{H}_A$ is determined by the cross-talk map $F : \{\Sigma_A^\omega : x \in \Sigma_A^\omega\} \rightarrow \mathcal{P}_\mathcal{B}$ defined as:

$$\forall x \in \Sigma_A^\omega, F(x, \Sigma_A^\omega) = (\Sigma_B^\omega, \mathcal{B}_B, \mu_B^F)$$

(68)

where $\mathcal{B}_B$ is the $\sigma$-algebra over $\Sigma_B$ constructed following Definition 2. If the probability space (See Lemma 7) induced by $\mathcal{H}_B$ is $(\Sigma_B^\omega, \mathcal{B}_B, \mu_B^F)$, then the cross-talk map is required to satisfy the following consistency criterion:

$$F(\Sigma_A^\omega) = (\Sigma_B^\omega, \mathcal{B}_B, \mu_B^F)$$

(Consistency)

Additionally, we assume that the cross-talk map is ergodic in the sense, that if $F(x, \Sigma_A^\omega) = (\Sigma_B^\omega, \mathcal{B}_B, \mu_B^F)$, $F(x, \Sigma_A^\omega) = (\Sigma_B^\omega, \mathcal{B}_B, \mu_B^F)$, then:

$$\forall x, y, z \in \Sigma_A^\omega, \lim_{|l| \rightarrow \infty} \|F^l(x, \Sigma_A^\omega) - F^l(y, \Sigma_A^\omega)\| = 0$$

(69) (Ergodicity)
i.e., the effect of some initial segment $x$ vanishes in the limit.

The cross-talk map induces the notion of the cross-derivative.

**Definition 15** (Cross-talk). Given two stationary ergodic QSPs $H_A, H_B$ over finite alphabets $\Sigma_A, \Sigma_B$ respectively, and the cross-talk map $F$, the cross-derivative $\phi^A_{\omega, x} H_B$ at $x \in \Sigma_A^*$ is a probability distribution over $\Sigma_B$ such that if $\phi^A_{\omega, x} H_B = (p_1, \ldots, p_i, \ldots)^T$, then the next symbol in $H_B$ is $\sigma_i$ with probability $p_i$, given that the string transpired in $H_A$ is $x$.

**Lemma 8** (Explicit Expression For Cross-talk). Given stationary ergodic QSPs $H_A, H_B$ over finite alphabets $\Sigma_A, \Sigma_B$ respectively, the cross-talk map $F$, and assuming $H_B$ has a PFSA representation $(Q_B, \Sigma_B, \sigma_0, \delta_B, \pi_B)$, we have:

$$\forall \sigma_i' \in \Sigma_B, \phi^A_{\omega, x} H_B|_{\sigma} = \sum_{r \in \Sigma_A^*} \mu^F(r \Sigma_A^*) \pi_B([r], \sigma_i')$$

*(Proof:)* For any $\tau \in \Sigma_A^*$, $\mu^F(r \Sigma_A^*)$ is the probability that $\tau$ transpired in $H_B$ given a string $x \in \Sigma_A^*$. Recalling that the terminal state or the equivalence class corresponding to $\tau$ is denoted by $[\tau]$, we note that the probability of generating $\sigma' \in \Sigma_B$ after $\tau$ is given by $\pi_B([\tau], \sigma_i')$. The result follows from noting that the $i$th entry of the cross-talk derivative at $x$ is the expected probability of generating $\sigma_i'$ next in $H_B$.

**Corollary 3** (To Lemma 8). The cross-derivative at the empty string may be expressed as:

$$\phi^A_{\omega, x} H_B|_{\sigma} = \varphi^A_{\omega, x} \pi_B$$

where $\varphi^A_{\omega, x}$ is the unique stationary distribution on the states of a PFSA representation for $H_B$.

*(Proof:)* Using the expression given by Lemma 8 we have:

$$\forall \sigma_i' \in \Sigma_B, \phi^A_{\omega, x} H_B|_{\sigma} = \sum_{r \in \Sigma_A^*} \mu^F(r \Sigma_A^*) \pi_B([r], \sigma_i')$$

$$= \sum_{r \in \Sigma_A^*} \mu^F(r \Sigma_A^*) \pi_B([r], \sigma_i')$$

(Using consistency of $F$, see Definition 14)

$$= \sum_{\tau \in \Sigma_A^*} \Pr([\tau]) \pi_B([r], \sigma_i') = \varphi^A_{\omega, x} \pi_B$$



**Definition 16** (Probabilistic Cross-Nerode Equivalence Relation). Given stationary ergodic QSPs $H_A, H_B$ over finite alphabets $\Sigma_A, \Sigma_B$ respectively, and the cross-talk map $F$, the cross-Nerode equivalence on $\Sigma_A^*$, denoted as $\sim^N_{H_B}$, is defined as:

$$\forall x, y \in \Sigma_A^*, x \sim^N_{H_B} y \quad \text{if} \quad \forall \tau \in \Sigma_A^*, \phi^A_{\omega, \tau} H_B = \varphi^A_{\omega, \tau}$$

Clearly, the cross-Nerode equivalence is right-invariant, i.e.,

$$\forall x, y \in \Sigma_A^*, x \sim^N_{H_B} y \Rightarrow \forall z \in \Sigma_A^*, xz \sim^N_{H_B} yz$$

which induces a notion of states, in the sense that if two strings are equivalent, we can forget which one was the actual history. This leads us to the notion of cross-probabilistic finite state automata as logical machines to represent cross-dependencies.

### 4.1 Crossed Probabilistic Finite State Automata (XPFSAs)

A crossed automata has an input alphabet and an output alphabet, and the idea is to model a finite state probabilistic transducer, that maps strings over the input alphabet to a distribution over set of finite strings over the output alphabet. Recall that these alphabets need not be identical with respect to their elements or their cardinalities. Formally, we define:

**Definition 17** (Crossed Probabilistic Finite State Automata). A crossed probabilistic finite state automaton (XPFA) is a 4-tuple $G = (Q, \Sigma, \delta, \pi)$, where $Q$ is a finite set of states, $\Sigma$ is a finite alphabet of symbols (known as the input alphabet), $\delta : Q \times \Sigma \to Q$ is the recursively extended transition function, $\Sigma'$ is a finite output alphabet with possibly $\Sigma \neq \Sigma'$, and $\pi : Q \times \Sigma' \to [0,1]$ is the output morph function parameterized by the output alphabet $\Sigma'$. In particular, $\pi(q, \sigma')$ is the probability of generating $\sigma' \in \Sigma'$ from a state $q \in Q$, and hence: $\pi(q) \equiv \Sigma_{\sigma' \in \Sigma'} \pi(q, \sigma') = 1$.

A XPFA with a marked initial state $q_0 \in Q$, is an initial-marked XPFA, which is described by the augmented quintuple $(Q, \Sigma, \delta, \pi, q_0)$.

**Lemma 9** (Cross-Nerode Equivalence to initial-marked XPFA). A cross-Nerode equivalence relation with finite index may be encoded by a XPFA.

*(Proof:)* For stationary ergodic QSPs $H_A, H_B$ over finite alphabets $\Sigma_A, \Sigma_B$ respectively, let $Q$ be the set of equivalence classes of the finite index cross-Nerode relation $\sim^N_{H_B}$ (Definition 16), and noting that $|Q| < \infty$, define functions $\delta : Q \times \Sigma_A \to Q$, $\pi : Q \times \Sigma_B \to [0,1]$ as:

$$\forall x \in \Sigma_A^*, \delta([x], \sigma) = [x \sigma]$$

(75a)

$$\forall x \in \Sigma_A^*, \pi([x], \sigma_i') \in \Sigma_B, \pi([x], \sigma_i') = \phi^A_{\omega, x} H_B [\sigma, \sigma_i']$$

(75b)

where we extend $\delta$ recursively to $y = x \sigma x' \in \Sigma_A^*$ as:

$$\delta(q, x \sigma x') = \delta(\delta(q, x), x')$$

(76)

Denoting $[\lambda]$ as $q_0$, we have an encoding for $\sim^N_{H_B}$ as a initial-marked XPFA $(Q, \Sigma, \delta, \pi, q_0)$.

Using the same argument from ergodicity as used in eliminating the initial making for PFSAs, we note that $q_0$ can be dropped without any loss of information. Later we argue that XPFSAs can be encoded as a Markov chain to a strong Markov chain, with strongly connected graphs.

Figure 3 illustrates the differences between PFSAs and XPFSAs. Note that inter-state transitions have generation probabilities in addition to symbol labels in the PFSAs, while in the XPFSA the transitions are labeled with only symbols from the input alphabet. The XPFSAs on the other hand have an output distribution over each state. This output distribution is over the output alphabet, and as shown in Figure 3 plates B and C, the size of the output alphabet (or its elements) may be different from that of the input alphabet.

4.1.1 *Specific cases: No Dependence & Identical Sample Paths*

Next we investigate some specific dependencies that may arise between stationary ergodic processes. The first case is when there is no dependence, e.g., when the evolution of $H_B$ cannot be predicted to any degree from a knowledge of $H_A$ evolution.

**Theorem 5** (XPFA Structure: First Result). For stationary ergodic QSPs $H_A, H_B$ over finite alphabets $\Sigma_A, \Sigma_B$ respectively, the following statements are equivalent:

1. $\forall x, y \in \Sigma_A^*, x \sim^N_{H_B} y$
2. $\forall x \in \Sigma_A^*, \phi^A_{\omega, x} H_B = v$ where $v$ is a constant vector
3. $\forall x \in \Sigma_A^*, \phi^A_{\omega, x} H_B = \varphi^A_{\omega, x} \pi_B$

*(Proof:)* 1) $\Rightarrow$ 2): Let $x, y \in \Sigma_A^*$. From Definition 16 we have:

$$x \sim^N_{H_B} y \Rightarrow \forall z \in \Sigma_A^*, xz \sim^N_{H_B} yz$$

and using 1) we conclude that $\phi^A_{\omega, x} H_B$ must be a constant vector for all $x \in \Sigma_A^*$.

1) $\Rightarrow$ 2): Follows from Definition 16.

3) $\Rightarrow$ 2): Trivial.
Let the $k^{th}$ symbol in the streams be represented as $s^A_k, s^B_k$. Fix $n \in \mathbb{N}$, and consider the random vectors $V \in \{s^A_1, \ldots, s^A_n, s^B_1, \ldots, s^B_n\}$, $W \in \{s^A_1, \ldots, s^B_n\}$. Also, let $Z_n$ denote the random variable for the $n^{th}$ symbol in $s^B$. Then, independence implies:

$$\forall x \in \Sigma^*_A, z \in \Sigma^*_B, \sigma' \in \Sigma^B, \quad Pr(V = x, W = z, Z_n = \sigma') = \Pr(V = x) \Pr(W = z, Z_n = \sigma')$$

(79)

Let a PFSAs description of $\mathcal{H}_A$ be $(Q, \Sigma^*_A, \delta, \pi^A)$. Assuming the canonical representation for the ergodic process $\mathcal{H}_B$, without loss of generality, we fix the initial state as the stationary distribution $\pi^B_0$. Then, by marginalizing out $W$, we get:

$$\forall x \in \Sigma^*_A, \sigma' \in \Sigma^B, \quad Pr(V = x, Z_n = \sigma') = \Pr(V = x) \sum_{q \in Q} \pi^B_{q} \pi^A(q, \sigma')$$

(80)

which then implies that:

$$\forall x \in \Sigma^*_A, \pi^{A, B}_x = \pi^B_0 \pi^A_x$$

(81)

Similarly, using the argument from $\mathcal{H}_B$ to $\mathcal{H}_A$, we get:

$$\forall y \in \Sigma^*_B, \pi^{B, A}_{y} = \pi^B_y \pi^A_{y}$$

(82)

which then completes the proof using Lemma 5.

**Lemma 11 (Unidirectional Dependence ≠ Independence).** There exist independent stationary ergodic QSPs $\mathcal{H}_A, \mathcal{H}_B$ over finite alphabets $\Sigma_A, \Sigma_B$ respectively, such that: $\forall x, y \in \Sigma^*_A, x \sim_{\mathcal{H}_A} y$, i.e., the minimal XPFSA from $\mathcal{H}_A$ to $\mathcal{H}_B$ has a single state.

**Proof:** We give an explicit example. Consider the processes $\mathcal{H}_A, \mathcal{H}_B$ over a binary alphabet $\{0, 1\}$ generating sample paths $s^A, s^B$ respectively via the following recursive rules (where $s^A_k, s^B_k$ are the symbols at step $k$):

$$s^B_0 = 0, s^A_0 = 0$$

(83)

$$Pr(s^A_{k+1} = 0 | s^A_k = 0) = 0.8, Pr(s^A_{k+1} = 1 | s^A_k = 0) = 0.2$$

(84)

$$Pr(s^B_{k+1} = 1 | s^B_k = 1) = 0.2, Pr(s^B_{k+1} = 1 | s^B_k = 1) = 0.8$$

(85)

$$Pr(s^B_k = 0 | s^A_k \in \{0, 1\}) = 0.5, Pr(s^B_k = 1 | s^A_k \in \{0, 1\}) = 0.5$$

(86)
It is immediate from Eq. (59) that $\forall x, y \in \Sigma^+, x \sim^H y$, and hence it follows from Lemma 5 that the minimal XPFSAs $H_A$ and $H_B$ have a single state. And since the current symbol in $s^d$ dictates the distribution of the next symbol in $s^t$, it is also immediate that the processes are not independent.

**Lemma 12** (Transition From Stationary Distribution). Let $G = (Q, \Sigma, \delta, \pi)$ be a PFSA representation for a stationary ergodic QS. If $G$ is distributed over its states as its stationary distribution $\pi$, and the next symbol is generated according to the distribution $\phi_\sigma \Pi$, then the next expected state distribution remains unaltered.

Proof: Let $\psi = \phi_\sigma \Pi$. Then the next state distribution $\phi'$, may be computed using the $|Q| \times |Q|$ transformation matrices $\Gamma_\sigma, \sigma \in \Sigma$ (See Definition 7) as:

$$\phi' = \phi_\sigma \sum_{j=1}^{n_0} \Gamma_\sigma v_j = \phi_\sigma \sum_{j=1}^{n_0} \phi_i j \sum_{i=1}^{n_1} \Gamma_\sigma \Pi_{i j}$$

(87)

Since $\sum_i \Gamma_\sigma = \Pi$, and $\forall j, \sum_i \Pi_{i j} = 1$, and $\sum_{j=1}^{n_0} \phi_i j = 1$, we conclude:

$$\phi' = \phi_\sigma \sum_{j=1}^{n_0} \phi_i j \Pi = \phi_i \Pi = \psi$$

(88)

which completes the proof.

**Lemma 13** (Condition For Trivial XPFSAs To Imply Independence). For stationary ergodic QSs $H_A, H_B$ over finite alphabets $\Sigma_A, \Sigma_B$ respectively, if we have:

$$\left( \forall x, y \in \Sigma_A^+, x \sim^H y \right) \land \left( \forall x', y' \in \Sigma_B^+, x' \sim^H y' \right)$$

(89)

then $H_A$ and $H_B$ are independent.

Proof: To assign explicit labels to the sequences of random variables in the processes under consideration, let $H_A = (W^{a_1}, H_B = (W^{b_1}), k \in \mathbb{N}$. For some arbitrary fixed $x, t \in \mathbb{N}$, satisfying $s \leq t$, let $H_A = (W^{a_1}, H_B = (W^{b_1}), k \in \mathbb{N}$, i.e., $H_A, H_B$ are right-translated variants of the processes $H_A, H_B$ respectively. We assume without loss of generality that the initial state for the canonical representations of the processes $H_A, H_B$ are $\phi_{a_1}^{\sigma}, \phi_{b_1}^{\sigma}$ (stationary distributions over the respective causal states, see Definition 8) respectively.

We claim that:

$$\forall x \in \Sigma_A, \phi_{a_1}^{\sigma, H_A} = \phi_{b_1}^{\sigma} \Pi_B$$

(90)

To establish this claim, we recall that the definition of crossed-derivative from one process to another has no reference to the transpired corresponding string in the second process. In other words, we marginalize out the transpired string in the second process. Since $H_B$ is assumed to be initialized at the stationary distribution $\phi_{b_1}^{\sigma}$, we conclude that marginalizing over all strings in $H_B$ that can transpire for some $x \in \Sigma_A$, the expected state is still $\phi_{b_1}^{\sigma}$ at $k = s$. Since the first conjunctive term in Eq. (89) implies that:

$$\forall x \in \Sigma_A, \phi_{a_1}^{\sigma, H_A} = \phi_{b_1}^{\sigma} \Pi_B$$

(91)

it follows that the expected state for $H_B$ at $k = s + 1$ is still $\phi_{b_1}^{\sigma}$ (Using Lemma 12). Continuing to marginalize of all sequences that may transpire between $k = s + 1$ and $k = t$, we conclude that the state at $k = t$ is still $\phi_{b_1}^{\sigma}$, and hence the next symbol will be distributed as $\phi_{b_1}^{\sigma} \Pi_B$. This establishes Claim A.

Next we claim that:

$$\forall x \in \Sigma_B, \phi_{b_1}^{\sigma, H_B} = \phi_{b_1}^{\sigma} \Pi_A$$

(92)

which follows immediately by noting that if $x = x_1 \cdots x_t \cdots x_n = y_{x_{s+1}} \cdots x_n$, then it follows from the second conjunctive term in Eq. (89):

$$\forall y = x_1 \cdots x_t \in \Sigma_B, \phi_{b_1}^{\sigma, H_B} = \phi_{b_1}^{\sigma} \Pi_A$$

(93)

and that the future symbols $x_{s+1} \cdots x_n$ do not affect the next-symbol distribution at $k = s$.

Also, note that as before, when we are computing $\phi_{b_1}^{\sigma, H_B}$, we can marginalize over all strings of length $s$ that occur in $H_B$, implying that the expected state at $k = s$ is $\phi_{b_1}^{\sigma}$.

Using claims A and B, and the fact that the expected states at $k = s$ and $k = t$ for the the processes $H_A', H_B'$ are $\phi_{a_2}^{\sigma}$ and $\phi_{b_2}^{\sigma}$ respectively, we conclude that:

$$\forall \sigma_i \in \Sigma_A, \sigma_j \in \Sigma_B,$$

$$\Pr[\Psi_i = \sigma_i, \Psi_j = \sigma_j] = \phi_{a_2}^{\sigma} \Pi A \phi_{b_2}^{\sigma} \Pi B = \Pr[\Psi_i = \sigma_i] \Pr[\Psi_j = \sigma_j]$$

(94)

which establishes the following:

$$\forall x, t \in \mathbb{N}, W^{a_1}, W^{b_1}$$

are pairwise independent

(95)

Finally, we use induction to complete the proof. We consider a sequence $k_1, \cdots, k_n$ with $\forall i, k_i \in \mathbb{N}$. For our induction basis, we note that claim C implies that $W^{a_1}, W^{b_1}$ are pairwise independent. As our induction hypothesis, let the random vectors $W^{a_1}, \cdots, W^{a_n}$ and $W^{b_1}, \cdots, W^{b_n}$ be independent. To conclude the proof, we argue:

$$\Pr[\Psi_i = \sigma_i] \Pr[\Psi_j = \sigma_j]$$

(96)

This completes the proof.

**Theorem 6** (Directional (In)Dependence). For stationary ergodic QSs to be independent, it is necessary and sufficient for the minimal XPFSAs in both directions to have a single state.

Proof: Follows immediately from Lemmas 10, 11, and 13.

Theorem 7 and the lemmas that build up to it, establish that XPFSAs capture a notion of directional dependence, and are well-suited to determine the directional causality flow between different processes. While the XPFSAs are generative models, it is useful to have a scalar quantification of the degree of directional dependence.

### 4.1.3 Degree Of Directional Dependence

The binary operation of composition on the space of probabilistic automata was introduced in the first author’s earlier work [17] for initial marked PFSA. We modify the definition to apply to PFSA representations for ergodic stationary QSs, where the initial state is unimportant.

**Definition 19** (Synchronous Composition Of Probabilistic Automata).

Let $G = (Q, \Sigma, \delta, \pi)$ be a PFSA representation of a stationary ergodic QS. Let $H = (Q', \Sigma, \delta')$ represent a strongly connected directed graph such that $Q'$ is the set of nodes, and $\forall q_i, q_j \in Q'$, there is a directed edge $q_i \rightarrow q_j$, labeled with $\sigma \in \Sigma$, if and only if $\delta'(q_i, \sigma) = q_j$. Let $G' = (Q \times Q', \Sigma, \delta', \pi')$ be a PFSA where the relevant functions are defined as:

$$\forall q_i \in Q, q_i_1 \in Q', \sigma \in \Sigma, \{ \delta'(q_i, q_i_1, \sigma) = (\delta(q_i, \sigma), \delta'(q_i, \sigma)) \}$$

(97)

Then the synchronous composition of $G, H$, denoted as $G \otimes H$, is any strongly connected component of $G'$.

We show that Definition 19 is consistent, in the sense that any two strongly connected components of $G'$ is structurally isomorphic.

**Lemma 14** (Well-definedness Of Synchronous Composition). Let $G^{a_1}, G^{a_2}$ be two strongly connected components of $G'$, as introduced in the course of Definition 19. Then, we have:

1. $G^{a_1}$ and $G^{a_2}$ are structurally isomorphic.
2) $G^\sigma; i = 1, 2$ encodes a refinement of the probabilistic Nerode relation encoded by $G$.

Proof: To establish statement 2), we must show that $G^\sigma$ is a non-minimal realization of the Nerode relation encoded by $G$, for any choice of initial state. To see this, choose a state $q_0 \in Q$, and augment $G$ to an initial-marked PFSA $(Q, \Sigma, \delta, \overline{\pi}, q_0)$. Also, choose a state $(q_0, q_0') \in Q \times Q'$, and augment $G^\sigma$ as $(Q \times \pi, \Sigma, \delta^\sigma, \overline{\pi}^\pi, (q_0, q_0'))$.

Then, it is immediate that:

$$\forall x, y \in \sum^\pi (\delta((q_0, q_0'), x) = \delta((q_0, q_0'), y) \Rightarrow \delta((q_0, x) = \delta((q_0, y))$$

(97)

This establishes statement 2).

Next, consider the graph for the PFSA $G^\sigma$, and augment it with a new morph function $\overline{\pi}'$, so as to get a PFSA $G'' = (Q \times \pi', \Sigma, \delta', \overline{\pi}')$, such that each row of $G''$ is distinct. It follows that no state in $G''$ may be merged with another, since for any two states $q, q' \in Q \times \pi'$, and any $\sigma \in \Sigma$, we have by construction: $\overline{\pi}'(q, \sigma) \neq \overline{\pi}'(q', \sigma)$.

Since, $H$ is strongly connected, $G''$ represents some specific probabilistic Nerode equivalence on $\sum^\pi$ (Note in contrast, if $H$ had multiple components, then the choice of the initial state might be important). Let the Nerode relation, corresponding to the stationary ergodic QSP encoded by $G''$, be denoted as $\sim_{G''}$.

Now, consider two strongly connected components $G_1, G_2$ for $G''$, with state sets $Q_1 \subseteq Q \times \pi', Q_2 \subseteq Q \times \pi'$. Since Theorem I establishes that strong components of PFSA are realizations of the same Nerode relation encoded by the full model, we conclude that $G_1$ and $G_2$ are both encodings of $\sim_{G''}$, i.e. there exists a map $\mathcal{H}_1 : Q_1 \rightarrow \mathcal{E}_1; \mathcal{H}_2 : Q_2 \rightarrow \mathcal{E}_2$, where $\mathcal{E}_1$ is the set of equivalence classes of $\sim_{G''}$. We note that it is immediate that $\mathcal{H}_1, \mathcal{H}_2$ are surjective. From definition of the Nerode equivalence, it also follows that no two states can map to the same equivalence class (to avoid merging), implying that $\mathcal{H}_1, \mathcal{H}_2$ are injective as well, implying that the inverse maps $\mathcal{H}_1^{-1}; \mathcal{E}_1 \rightarrow Q_1; \mathcal{H}_2^{-1}; \mathcal{E}_2 \rightarrow Q_2$ are well-defined. Now, we construct maps $\xi : Q_1 \rightarrow \mathcal{E}_1; \xi' : Q_2 \rightarrow \mathcal{E}_2$ as follows:

$$\forall q \in Q_1, \xi(q) = \mathcal{H}_1^{-1}(\mathcal{H}_1(q)) \quad (98)$$

$$\forall q \in Q_2, \xi'(q) = \mathcal{H}_2^{-1}(\mathcal{H}_2(q)) \quad (99)$$

It follows that:

$$\forall q \in Q_1, \xi'(\xi(q)) = \mathcal{H}_1^{-1}(\mathcal{H}_1(\xi'(q))) = q \quad (100)$$

implying $\xi$ is bijective. Since $G_1, G_2$ are components of $G''$, we note:

$$\forall \sigma \in \Sigma, q, q' \in Q \subseteq Q \times \pi'$$

$$\delta'(q, \sigma) = \mathcal{H}_1^{-1}((q, \mathcal{E}_1(q))) \Rightarrow e(\delta'(q, \sigma)) = \mathcal{H}_1^{-1}((q, \mathcal{E}_1(q)))$$

$$\Rightarrow \mathcal{H}_2^{-1}((q, \mathcal{E}_1(q))) = \mathcal{H}_2^{-1}((q, \mathcal{E}_2(q)))$$

(101)

Similarly, assuming the probability measure on $\sum^\pi$ encoded by $G''$ is $\mu$, we also have:

$$\forall \sigma \in \Sigma, q, \mu(q, \sigma) = \mathcal{H}_2^{-1}((q, \mathcal{E}_2(q)))$$

and, also:

$$\forall \sigma \in \Sigma, q, \mu(q, \sigma) = \mathcal{H}_2^{-1}((q, \mathcal{E}_2(q)))$$

which implies:

$$\forall \sigma \in \Sigma, q, \mu(q, \sigma) = \frac{\mu(q, \sigma \sigma)}{\mu(q, \Sigma^\pi)}$$

(103)

Hence, $G_1, G_2$ are structurally isomorphic. Noting that the morph $\overline{\pi}'$ is arbitrary completes the proof.

Next we introduce projective composition. Again, a slightly different version was introduced in the authors’ earlier work[35].

**Definition 20** (Projective Composition). For a given PFSA $G = (Q, \Sigma, \delta, \overline{\pi})$, and a strongly connected directed graph $H = (Q', \Sigma, \delta')$, such that $Q'$ is the set of nodes, and $\forall q, q' \in Q'$, there is a directed
edge \( q' \xrightarrow{\delta'} q' \), labeled with \( \sigma \in \Sigma \), if and only if \( \delta'(q', \sigma) = q' \), the projective composition \( G \boxtimes H = (Q', \Sigma, \delta', \overline{\pi}') \) is a PFSA with:

\[
\forall q' \in Q', \sigma \in \Sigma, \\
\pi'(q', \sigma) = \begin{cases} \\
\sum_{(q,q') \in Q'^2} \pi''((q, q'), \sigma) \phi''_{(q, q')} \bigg|_{q'=q} \\
\sum_{(q,q') \in Q'^2} \phi''_{(q, q')} \bigg|_{q'=q} \\
\end{cases} \tag{105}
\]

where \( G \otimes H = (Q', \Sigma, \delta', \overline{\pi}') \) , and \( \phi''_{(q, q')} \) is the corresponding stationary distribution on \( Q'' \).

Note that synchronous and projective compositions are defined to operate on a pair of arguments, the first of which is a PFSA and the second is a strongly connected graph with edges labeled by symbols from the same alphabet. However, we can extend them as binary operators on the space of strongly connected PFSA on a fixed alphabet, using the graph of the second PFSA as the second argument for the operators. Thus, it makes sense to talk about \( G \otimes G \otimes H, G \otimes G \otimes H \) where \( G, H \) are PFSA with strongly connected graphs. Indeed, one can show easily that, for any such PFSA \( G, H \):

\[
G \otimes G = G \\
G \otimes G = G \\
(G \otimes H) \otimes H = G \otimes H \\
\]

Additionally, the projective composition preserves the projected distribution.

**Def 21 (Projected Distribution).** Given a PFSA \( G \) encoding the probability space \((\Sigma^w, \mathcal{B}, \mu_\sigma)\), and a PFSA \( H = (Q', \Sigma, \phi', \overline{\pi}') \), the projected distribution \( [G]_{\mu_\sigma} \) of \( G \) with respect to \( H \) is a vector \( \phi \in [0,1]^{|Q'|} \), such that:

\[
\forall j \in \{1, \ldots, |Q'|\}, \phi_j = \sum_{x \in \Sigma} \mu_\sigma(x) \theta_j^w \\
\tag{109}
\]

for any choice of initial state in \( G \), and where \( \theta_j^w \) is the equivalence class for the transition equivalence (See Lemma 3) corresponding to state \( q_j \in Q_j \), again for any choice of initial state in \( H \).

We note \( [G]_{\mu_\sigma} \) is always an “probability vector”, i.e.,

\[
\forall j \in \{1, \ldots, |Q'|\}, [G]_{\mu_\sigma} \geq 0 \text{ and } \sum_{j=1}^{|Q'|} [G]_{\mu_\sigma} = \sum_{x \in \Sigma} \mu_\sigma(x) = 1 \\
\tag{110}
\]

**Lemma 15 (Projected Distribution Well-defined-ness & Invariance).** For PFSA \( P \) and \( G \) encoding stationary ergodic QSPs over the same alphabet:

1) \( [G]_{\mu_\sigma} \) is independent of the choice of the initial states in Definition 21.

2) \( [G]_{\mu_\sigma} \) is the stationary distribution on the states of the projective composition of \( G \) with \( H \), i.e., we have:

\[
[G]_{\mu_\sigma} = [G \otimes H]_{\mu_\sigma} \\
\tag{111}
\]

**Proof:** We note that statement 2) implies statement 1) from ergodicity. To establish statement 2), we argue as follows: Let \( G = (Q, \Sigma, \delta, \overline{\pi}), H = (Q', \Sigma, \delta', \overline{\pi}') \), and also let \( G \otimes H = (Q', \Sigma, \delta', \overline{\pi}') \).

Let \( [G]_{\mu_\sigma} = \phi^\sigma \). Additionally, let the stationary distribution on the states of \( G \otimes H \) be denoted as \( \phi^\sigma \).

We claim \( \phi^\sigma \) is also a stationary distribution for \( G \otimes H \).

Denoting the measure encoded by \( G \) as \( \mu_\sigma \), and the equivalence class for the transitional equivalence corresponding to state \( q_j \in Q \) as \( \mathcal{E}(q_j) \), we note that:

\[
\phi^\sigma_j = \sum_{x \in \mathcal{E}(q_j) \cap \Sigma} \mu_\sigma(x) = \sum_{q \in Q} \phi''_{(q, q')} \\
\tag{112}
\]

where we have used the fact that states in \( G \otimes H \) are of the form \((q, q')\), with \( q \in Q, q' \in Q' \). The transition probability matrix \( \Pi'' \) for \( G \otimes H \) (each entry being the probability of transitioning from one state to another via possibly different symbols, in a single step) is defined as:

\[
\Pi''_{(q,q')}(\sigma) = \frac{\sum_{\sigma \sigma' \in \Sigma^o} \Pi''_{(q,\sigma')}(\sigma') \pi''_{(q', \sigma')} \bigg|_{q'=q}}{\sum_{\sigma \sigma' \in \Sigma^o} \pi''_{(\sigma', \sigma')} \bigg|_{\sigma'=q}} \\
\tag{113}
\]

and we set (assuming \( \phi^\sigma \) is a row-vector):

\[
v \cdot \phi^\sigma = v^\top \phi^\sigma \\
\tag{114}
\]

implying that we have:

\[
\forall q_j \in Q, v_k = \sum_{j=1}^{|Q|} \phi''_{(q_j, q_k)} \pi''_{(q, q')} \bigg|_{q'=q} \\
\tag{115}
\]

Since, \( \phi^\sigma \) is a stationary distribution for \( G \otimes H \), it follows:

\[
\forall q_j \in Q', v_k = \sum_{q \in Q} \phi''_{(q, q')} \pi''_{(q, q')} \bigg|_{q'=q} \\
\tag{116}
\]

which establishes that \( v = \phi^\sigma \), i.e., \( \phi^\sigma \) is a stationary distribution for \( G \otimes H \). By ergodicity, it follows that stationary distributions for both \( G \) and \( G \otimes H \) are unique, which completes the proof. \( \square \)

We are now ready to define the coefficient of causal dependence. We recall from Definition 15 that given two stationary ergodic QSPs \( \mathcal{H}_A, \mathcal{H}_B \) over finite alphabets \( \Sigma_A, \Sigma_B \), the cross-derivative \( \phi''_{(q, q')} \) at \( x \in \Sigma_A^o \) specifies the next-symbol distribution in \( \mathcal{H}_B, \) given the knowledge that the string transpired in \( \mathcal{H}_A \) is \( x \).

**Def 22 (Coefficient Of Causal Dependence).** Let \( \mathcal{H}_A, \mathcal{H}_B \) be stationary ergodic QSPS over finite alphabets \( \Sigma_A, \Sigma_B \) respectively. The coefficient of causal dependence of \( \mathcal{H}_B \) on \( \mathcal{H}_A \), denoted as \( \gamma^\sigma_{A \rightarrow B} \), is defined as the ratio of the expected change in entropy of the next symbol distribution in \( \mathcal{H}_B \) due to observations in \( \mathcal{H}_A \) to the entropy of the next symbol distribution in \( \mathcal{H}_B \) in the absence of observations in \( \mathcal{H}_A \), i.e., we have:

\[
\gamma^\sigma_{A \rightarrow B} = \frac{\mathbb{E}_{x \in \Sigma_A} \left( h\left( \phi''_{(q, q')}(x) \right) \right)}{h\left( \phi''_{(q, q')}(x) \right)} \\
\tag{117}
\]

where the entropy \( h(u) \) of a discrete probability distribution \( u \) is given by \( \sum u \log_2 u \). We assume that \( h \) is not a trivial process, producing only a single alphabet symbol, thus precluding the possibility that the denominator is zero.

**Lemma 16 (XPFSA to Coefficient of Causal Dependence).** For stationary ergodic QSPS \( \mathcal{H}_A, \mathcal{H}_B \) over alphabets \( \Sigma_A, \Sigma_B \), let the PFSA encoding the processes be \( A = (Q_A, \Sigma_A, \delta_A, h_A) \) and \( B = (Q_B, \Sigma_B, \delta_B, h_B) \) respectively. Also, let the XPFSA from \( \mathcal{H}_A \) to \( \mathcal{H}_B \) be \( B^A = (Q_A^B, \Sigma, \delta_A^B, h_B) \). Then, if \( Q_A^B = \{q_1, \ldots, q_m\} \), then we have:

\[
\gamma^\sigma_{A \rightarrow B} = \frac{\sum_{q \in Q^B} h\left( \phi''_{(q, q')} \right) \left( \mathbb{E}_{q \in \Sigma} h\left( \phi''_{(q, q')} \right) \right) \bigg|_{q=q} \bigg|_{q'=q}}{h\left( \phi''_{(q, q')} \right) \bigg|_{q=q} \bigg|_{q'=q}} \\
\tag{118}
\]

where \((\cdot, \cdot)\) is the standard inner product, and \( \phi''_{(q, q')} \) is the stationary distribution on the states of \( B \).

**Proof:** The denominator follows from Corollary 3 to Lemma 1. Let \( A \) encode the probability space \((\Sigma_A^w, \mathcal{B}, \mu)\). Then, we have:

\[
\mathbb{E}_{x \in \Sigma_A} h\left( \phi''_{(q, q')} \right) = \sum_{x \in \Sigma_A^w} \mu_\sigma(x) h\left( \phi''_{(q, q')} \right) \\
\tag{119}
\]
Recursive System Description
($s^x_A$, $s^x_B$ sample paths for $H_A, H_B$)

\[ s^0_A = 0, \quad s^0_B = 0 \]
\[ Pr(s^1_A = 0 | s^0_A = 0) = 0.8 \]
\[ Pr(s^1_A = 1 | s^0_A = 0) = 0.2 \]
\[ Pr(s^1_A = 0 | s^0_A = 1) = 1 \]
\[ Pr(s^1_A = 1 | s^0_A = 1) = 0.8 \]
\[ Pr(s^1_B = 0 | s^0_B = 0) = 0.2 \]
\[ Pr(s^1_B = 1 | s^0_B = 1) = 0.5 \]
\[ Pr(s^1_B = 1 | s^0_B = 0) = 0.5 \]

Coefficients of Dependence

\[ \gamma^A_B = 0 \]
\[ \gamma^B_A = 0.2781 \]  

Fig. 6. Example Processes With Uni-directional Dependence. For the system description tabulated above, we get the two self-models (plates A and B) which are single state PFSAs. It also follows that process $H_A$ cannot predict any symbol in process $H_B$, and we get the XPSFA from $A$ to $B$ as a single state machine as well (plate C). However, process $H_A$ is somewhat predictable by looking at $H_B$, and we have the XPSFA with two states in this direction (plate D). Note the tabulated coefficients of dependence in the two directions. Since for this example, $H_A$ is the Bernoulli-1/2 process with entropy rate of $I$ bit/letter, it follows that making observations in the process $H_B$ reduces the entropy of the next-symbol distribution in $H_A$ by 0.2781 bits.

Noting that the equivalence classes of the cross-Nerode equivalence $\sim_{H_B}$ correspond to elements in the set $Q^*_{H_B}$, we denote the equivalence class of strings in $\Sigma^*_A$ corresponding to state $q \in Q^*_{H_B}$ as $E(q)$. Then:

\[ \sum_{x \in \Sigma^*_A} \mu(x) x h(\phi^{H_A,H_B}_{H_A}(x)) = \sum_{q \in Q^*_{H_B}} \sum_{x \in E(q)} \mu(x) x h(\phi^{H_A,H_B}_{H_A}(x)) \quad (120) \]

We note that:

\[ \forall x \in E(q), \quad \phi^{H_A,H_B}_{H_A}(x) = \bar{\pi}^A_B(x) \cdot \phi^{H_A,H_B}_{H_A}(q) \quad (121) \]

and hence we have, using Definition 21 and Lemma 15:

\[ \sum_{q \in Q^*_{H_B}} \sum_{x \in E(q)} \mu(x) x h(\phi^{H_A,H_B}_{H_A}(x)) \]

\[ = \sum_{q \in Q^*_{H_B}} h(\bar{\pi}^A_B(q)) \left( \sum_{x \in \Sigma^*_A} \mu(x) x \right) \]

\[ = \sum_{q \in Q^*_{H_B}} h(\bar{\pi}^A_B(q)) \left( \sum_{x \in \Sigma^*_A} \mu(x) x \right) A_{H_B} = \gamma^A_B \quad (122) \]

\[ = \sum_{q \in Q^*_{H_B}} h(\bar{\pi}^A_B(q)) \left( \sum_{x \in \Sigma^*_A} \mu(x) x \right) B_{H_B} = \gamma^B_A \quad (123) \]

which completes the proof.

Theorem 7 (Properties of Coefficient Of Causal Dependence). For stationary ergodic QSPs $H_A, H_B$ over alphabets $\Sigma_A, \Sigma_B$, we have:

1) $\gamma^A_B \in [0, 1]$

2) $H_A$ and $H_B$ are independent if and only if $\gamma^A_B = \gamma^B_A = 0$.

Proof: We note that non-negativity of entropy implies:

\[ \frac{E_{x \in \Sigma^*_A} h(\phi^{H_A,H_B}_{H_A}(x))}{h(\phi^{H_A,H_B}_{H_A}(x))} \geq 0 \Rightarrow \gamma^A_B \geq 0 \quad (124) \]

For the upper bound, we note that by marginalizing out $x$ from $\phi^{H_A,H_B}_{H_A}$, we get:

\[ \phi^{H_A,H_B}_{H_A} = \sum_{x \in \Sigma^*_A} \phi^{H_A,H_B}_{H_A}(x) \]

\[ \Rightarrow \frac{E_{x \in \Sigma^*_A} h(\phi^{H_A,H_B}_{H_A}(x))}{h(\phi^{H_A,H_B}_{H_A}(x))} = \sum_{x \in \Sigma^*_A} \frac{h(\phi^{H_A,H_B}_{H_A}(x))}{h(\phi^{H_A,H_B}_{H_A}(x))} \quad (125) \]

Since entropy is concave, Jensen’s inequality [43] guarantees:

\[ E_{x \in \Sigma^*_A} h(\phi^{H_A,H_B}_{H_A}(x)) \leq h\left( E_{x \in \Sigma^*_A} \phi^{H_A,H_B}_{H_A}(x) \right) \Rightarrow \gamma^A_B \leq 1 \quad (126) \]

This establishes statement 1).

Next we note that:

\[ \gamma^A_B = 0 \Rightarrow E_{x \in \Sigma^*_A} h(\phi^{H_A,H_B}_{H_A}(x)) = h\left( E_{x \in \Sigma^*_A} \phi^{H_A,H_B}_{H_A}(x) \right) \quad (127) \]

\[ \Rightarrow \gamma^B_A = 0 \Rightarrow E_{x \in \Sigma^*_A} h(\phi^{H_A,H_B}_{H_A}(x)) = h\left( E_{x \in \Sigma^*_A} \phi^{H_A,H_B}_{H_A}(x) \right) \quad (128) \]

5 Algorithm GenESeSS: Self-model Inference

We construct an effective procedure to infer PFSAs $\mathcal{P}_H$ from a sufficiently long run from a QSP $H$, and a pre-specified $\epsilon > 0$. This section (Section 5) has largely appeared elsewhere [31], but is included for the sake of completeness.

5.1 Implementation Steps

The inference algorithm for PFSAs seeks similar symbolic derivatives (similar in the sense that infinity norm of the difference is within some pre-specified bound $\epsilon$), and “merges” string fragments at which the derivatives turn out to be similar, i.e. define them to reach the same state in the underlying model. This is more general to state splitting or state merging, since both processes are going on simultaneously: when we find a symbolic derivative that fails to match to any of the derivatives already encountered, we create a new state; while if we do find such a match, then we merge the two strings at which the derivatives are found to be similar. It is crucial that we first seek out an $\epsilon$-synchronizing string, and look at its right extensions to carry out the merge and split; which, due to the preceding theoretical development,
ensures that we are finding states of the underlying $\mathcal{P}_H$ within $\epsilon$ error in the infinity norm.

We call our algorithm “Generator Extraction Using Self-similar Semantics”, or GenESeSS which for an observed sequence $s$, consists of three steps:

1) Identification of e-synchronizing string $x_0$: Construct a derivative heap $D'(L)$ using the observed trace $s$ (Definition $\mathbb{[13]}$), and set $L$ consisting of all strings up to a sufficiently large, but finite, depth. We suggest as initial choice of $L$ as $\log_{|\Sigma|} 1/\epsilon$. In $L$ is sufficiently large, then the inferred model structure will not change for larger values. We then identify a vertex of the convex hull for $D_x$, via any standard algorithm for computing the hull $[43]$. Choose $x_0$ as the string mapping to this vertex.

2) Identification of the structure of $\mathcal{P}_H$, i.e., transition function $\delta$: We generate $\delta$ as follows: For each state $q$, we associate a string identifier $x_{q0} \in \mathcal{X}_\Sigma$, and a probability distribution $h_q$ on $\Sigma$ (which is an approximation of the $\tilde{\Pi}$-row corresponding to state $q$).

We extend the structure recursively:

a) Initialize the set $Q = \{q_0\}$, and set $x_{q0} = x_0$, $h_q = \phi(x_0)$.

b) For each state $q \in Q$, compute for each symbol $\sigma \in \Sigma$, find symbolic derivative $\delta(x_{q\sigma})$. If $|\delta(x_{q\sigma}) - h_q|_\infty \leq \epsilon$ for some $q' \in Q$, then define $\delta(q, \sigma) = q'$. If, on the other hand, no such $q'$ can be found in $Q$, then add a new state $q'$ to $Q$, and define $x_{q\sigma} = x_{q'\sigma}$, $h_q = \phi(x_{q'\sigma})$.

The process terminates when every $q \in Q$ has a target state, for each $\sigma \in \Sigma$. Then, if necessary, we ensure strong connectivity using $[45]$.

3) Identification of arc probabilities, i.e., function $\bar{\Pi}$: a) Choose an arbitrary initial state $q \in Q$.

b) Run sequence $s$ through the identified graph, as directed by $\delta$, i.e., if current state is $q$, and the next symbol read from $s$ is $\sigma$, then move to $\delta(q, \sigma)$. Count arc traversals, i.e., generate numbers $N_{q\sigma}$ where $q_i \rightarrow_{q_j}$ $q_k$.

c) Generate $\bar{\Pi}$ by row normalization, i.e., $\bar{\Pi}_{q\sigma} = N_{q\sigma}/(\sum_j N_{qj})$

Reported recursive structure extension algorithms $[33], [46]$ lack the e-synchronization step, and are restricted to inferring only synchronizable or short-memory models, or large approximations for long-memory ones.

5.2 Complexity Analysis & PAC Learnability

GenESeSS has no upper bound on the number of states; which is a function of the process complexity itself.

While $h_q$ (in step 2) approximates $\tilde{\Pi}$ rows, we find the arc probabilities via normalization of traversal count. $h_q$ only uses sequences in $x_{q\Sigma^*}$, while traversal counting uses the entire sequence $s$, and is more accurate.

We assume that the $\tilde{\Pi}$ rows corresponding to distinct states are separated in the sup norm by at least $\epsilon$. A PFSAs with distinct states may have identical rows corresponding to multiple states. However, not all rows can be identical, for then the states would collapse, and we would get a single state PFSAs. The proposed algorithm can be easily modified to address this issue; if two states have identical corresponding $\tilde{\Pi}$ rows, then they can be disambiguated from the multiplicity of outgoing transitions with identical labels; however we do not discuss this issue here.

Another issue is obtaining a strongly connected PFSAs, which can be ensured if before Step 2, we extract a strong component from the structure inferred in Step 1. This can be carried out efficiently using Tarjan’s algorithm $[45]$, which has $O(|Q| + |\Sigma|)$ asymptotic space and time complexity.

**Theorem 8 (Time Complexity).** Assuming $|s| > |\Sigma|$, the asymptotic time complexity of GenESeSS is:

$$\mathcal{T} = O\left(\frac{|s||\Sigma|}{\epsilon}\right)$$

**Proof:** Assuming $|s| > |\Sigma|$, we note that GenESeSS performs the following computations:

C1 Computation of a derivative heap by computing $\phi'(x)$ for $O(1/\epsilon)$ strings (Corollary $\mathbb{[1]}$), each of which involves reading the input $s$ and normalization to distributions over $\Sigma$, thus contributing $O(1/\epsilon \times (|s| + |\Sigma|)) = O(1/\epsilon \times |s|)$.

C2 Finding a vertex of the convex hull of the heap, which, at worst, involves inspecting $O(1/\epsilon)$ points (encoded by strings generating the heap), contributing $O(1/\epsilon \times |\Sigma|)$, where each inspection is done in $O(\Sigma)$ time.

C3 Finding $\delta$, involving computing derivatives at string-identifiers (Step 2), thus contributing $O(|Q| \times |\Sigma|)$.

C4 Identification of arc probabilities using traversal counts and normalization, done in time linear in the number of arcs, i.e. $O(|Q| \times |\Sigma|)$.

Summing the contributions, we have:

$$\mathcal{T} = O(1/\epsilon \times |s| + 1/\epsilon \times |\Sigma| + |Q| \times |s| + |Q| \times |\Sigma|)$$

$$= O\left(\left(1/\epsilon + |Q| \times |\Sigma|\right) \times |s|\right)$$

(135)

Noting that $|Q|$ is bounded by the maximum number of symbolic derivatives that may be distinguished, and hence by $1/\epsilon$, we conclude:

$$\mathcal{T} = O\left(\frac{|s||\Sigma|}{\epsilon}\right)$$

(136)

which completes the proof.

Finite probabilistic identification is referred to as Probably Approximately Correct learning $[30], [47], [48]$ (PAC-learning), which accepts a hypothesis that is not too different from the correct language with high probability. An identification method is said to identify a target language $L_*$ in the Probably Approximately Correct (PAC) sense $[30], [47], [48]$, if it always halts and outputs $L$ such that:

$$3\epsilon, \delta > 0, P(d(L_*, L) \leq \epsilon) \geq 1 - \delta$$

(137)

where $d(\cdot, \cdot)$ is a metric on the space of target languages. A class of languages is efficiently PAC-learnable if there exists an algorithm that PAC-identifies every language in the class, and runs in time polynomial in $1/\epsilon$, $1/\delta$, length of sample input, and inferred model size. We prove PAC-learnability of QSPs, by first establishing a metric on the space of probabilistic automata over $\Sigma$.

5.3 PAC Learnability Of QSPs

We first establish an appropriate metric to establish PAC-learnability of GenESeSS.

**Lemma 17** (Metric For Probabilistic Automata). For two strongly connected PFSAs $G_1, G_2$, let the symbolic derivative at $x \in \Sigma^*$ be denoted as $\phi_{G_1}(x)$ and $\phi_{G_2}(x)$ respectively. Then:

$$\Theta(G_1, G_2) = \sup_{s \in \Sigma^*} \left\{ \lim_{|s|, |s_0| \to \infty} \| \phi_{G_1}(s) - \phi_{G_2}(s) \|_\infty \right\}$$

(138)

defines a metric on the space of probabilistic automata on $\Sigma$.

**Proof:** Non-negativity and symmetry follows immediately. Triangular inequality follows from noting that $\| \phi_{G_1}(s) - \phi_{G_2}(s) \|_\infty$ is upper bounded by 1, and therefore for any chosen order of the strings in $\Sigma^*$, we have two $\epsilon_0$ sequences, which would satisfy the triangular inequality under the sup norm. The metric is well-defined since for any sufficiently long $s_1, s_2$, the symbolic derivatives at arbitrary $x$ are uniformly convergent to some linear combination of the rows of the corresponding $\tilde{\Pi}$ matrices.

Now, we can establish that the class of ergodic, stationary QSPs with a finite number of causal states is PAC-learnable.

**Theorem 9** (PAC-Learnability of QSPs). Ergodic, stationary QSPs for which the probabilistic Nerode equivalence has a finite index satisfies the following property:

For $\epsilon, \eta > 0$, and for every sufficiently long sequence $s$ generated by QSP $H$, GenESeSS computes $\mathcal{P}_H'$ as an estimate for $\mathcal{P}_H$ with:

$$Pr(\Theta(\mathcal{P}_H, \mathcal{P}_H') \leq \epsilon) \geq 1 - \eta$$

(139)
Asymptotic runtime is polynomial in $1/\epsilon, 1/\eta, |s|$. 

Proof: GenESeSS construction and Corollary 2 to Theorem 5 implies that, once the initial $e$-synchronizing string $x_0$ is identified, right extensions of $x$ (with non-zero probability of occurrence from the synchronized state) are $e'$-synchronizing where $e' = eC_0$, with $C_0 < \infty$ as defined in Eq. (53).

If the target QSP has $|Q|$ states, then $|Q|$ states need to be visited with right extensions of the computed $e$-synchronizing string $x$. Hence, for any $e'' > 0$, 

$$Pr(\Theta(P_H, P_0) \leq C_0 | e'' |) = 1 - Pr(\|\phi'(x_0) - \phi_{x_0}\|_\infty > e'')$$

$$= 1 - e^{-|\Theta(P_H, P_0)|/(\log 2)}$$

(Using Eq. (67)).

Thus, for any $\eta > 0$, if we have $|s| = O(C_0^{\log 2})$, then the required condition of Eq. (139) is met. Polynomial runtimes is established in Theorem 6.

Corollary 4 (To Theorem 9) Sample Complexity. The input length required for PAC-learning with GenESeSS is asymptotically linear in $1/\epsilon, 1/\eta, |s|$, but exponential in the number of causal states $|Q|$.

Proof: Immediate from Theorem 9.

Remark 2 (Sample Complexity). The exponential asymptotic dependence of the sample complexity on the number of causal states of the target QSP should not be interpreted as inefficiency. Unlike standard treatments of PAC learning, here we do not have a set of independent samples as training, but a single long input stream. Noting that an input $s$ is composed of an exponential number of subwords (summed over all lengths), the exponential dependence on $|Q|$ vanishes, if we treat this set of subsequences as the sample set. Thus, it is a matter of how one chooses to define the notion of sample complexity for this setting.

Remark 3 (Remark On Kearns’ Hardness Result). We are immune to Kearns’ hardness result [49], since $e > 0$ enforces state distinguishability [50], and furthermore, the restriction of our systems of interest to ergodic stationary dynamical systems, which produce termination-free traces, makes Kearns’ particular construction with parity function [59] inapplicable.

6 Algorithm xGenESeSS: Cross-model Inference

We note that the notion of structural isomorphism between PFSA (See Definition 2) extends naturally to XPFSA, with the output morph function in the latter playing the role of the morph function in the former. In particular, we note that the assumed ergodicity of the processes and of the cross-talk map (See Definition 14), implies that we have a result similar to Theorem 1, namely that XPFSA have unique minimal realizations, which are strongly connected.

Lemma 18 (Existence Of Unique Strongly Connected Minimal XPFSA Realization). For stationary ergodic QSPs $H_a, H_b$ over alphabets $\Sigma_a, \Sigma_b$, if the probabilistic cross-Nerode relation $\gamma_{H_a}$ on $\Sigma_a^*$ (with respect to a consistent, ergodic cross-talk map, see Definition 14) has a finite index, then it has a strongly connected XPFSA generator unique up to structural isomorphism.

Proof: The argument is identical to that in Theorem 1 using the construction described in Lemma 9.

$e$-synchronization plays an important role in GenESeSS. A corresponding notion of synchronization is necessary for inferring XPFSA. However, since XPFSA model dependence between processes, and not the processes themselves, the notion $e$-synchronization in this case cannot be based solely on the XPFSA structure or its output morph. Specifically, since the transitions in a XPFSA lack the generation probabilities, it does not make sense to talk about synchronization in the same sense as of a PFSA. However, synchronization is still necessary to ensure that we infer the XPFSA states, and not distributions on them. We need induced cross-distributions, i.e., distributions on the XPFSA states given a observed string in the first process, to make the notion of synchronization well-defined.

Definition 23 (Induced Cross-Distribution). Given stationary ergodic QSPs $H_a, H_b$ over alphabets $\Sigma_a, \Sigma_b$, a PFSA generator $G_a$ for $H_a$, and the minimal XPFSA $B^x = (Q^x, \Sigma_a, \delta^x, \pi_{x_a})$ from $H_a$ to $H_b$, each $x \in \Sigma_a^*$ induces a distribution $\rho_{x_a}^{H_a, \pi_{x_a}}$ over $Q_a$ defined recursively as:

$$\rho_{x_a}^{H_a, \pi_{x_a}} = \left[ G_a \otimes B^x \right] \pi_{x_a}$$

where we assume $\rho_{x_a}^{H_a, \pi_{x_a}}$ is a row vector, and $\Gamma_{B^x}$ is the symbol-specific transformation matrix for $B^x$ using the output morph as the function (See Definition 7).

Lemma 19 (Induction of Cross-Distribution). Given stationary ergodic QSPs $H_a, H_b$ over alphabets $\Sigma_a, \Sigma_b$, a PFSA generator $G_a$ for $H_a$, and the minimal XPFSA $B^x = (Q^x, \Sigma_a, \delta^x, \pi_{x_a})$ from $H_a$ to $H_b$, the induced cross-distribution $\rho_{x_a}^{H_a, \pi_{x_a}}$ satisfies:

$$\forall x \in \Sigma_a^*, \forall s_0 \in \Sigma_a \rho_{s_0}^{H_a, \pi_{x_a}} = \left( E \phi_{s_0}^x \right)_{|s_0|}$$

assuming as before that $\rho_{s_0}^{H_a, \pi_{x_a}}$ is a row vector.

Proof: Denoting the probability space induced by $H_a$ as $(\Sigma_a^*, \mathbb{B}, \mu_a)$, and the equivalence class corresponding to state $q \in Q_a$ as $E(q)$, we note:

$$E \phi_{s_0}^{H_a, \pi_{x_a}} = \sum_{y \in \Sigma_a^*} \mu_a(y) \rho_{y}^{H_a, \pi_{x_a}} = \sum_{y \in \Sigma_a^*} \mu_a(y) \left( \sum_{q \in E_y} \pi_{x_a}^{H_a}(q, \cdot) \right)$$

(142)

Finally, noting that Definitions 21 and 23 imply:

$$\rho_{s_0}^{H_a, \pi_{x_a}} = \sum_{y \in \Sigma_a^*} \mu_a(y) \left( \sum_{q \in E_y} \pi_{x_a}^{H_a}(q, \cdot) \right)$$

(143)

completes the proof.

Definition 24 ($e$-Synchronization of XPFSA). For stationary ergodic QSPs $H_a, H_b$ over alphabets $\Sigma_a, \Sigma_b$, and a XPFSA $B^x = (Q^x, \Sigma_a, \delta^x, \pi_{x_a})$ from $H_a$ to $H_b$, a string $x_0 \in \Sigma_a^*$ is $e$-synchronizing with respect to $B^x$, if

$$\exists q \in Q_a \left\| E \phi_{s_0}^{H_a, \pi_{x_a}} - \pi_{x_a}(q, \cdot) \right\|_\infty \leq e$$

(144)

The next result reduces the computation of an $e$-synchronizing string for a XPFSA to that for a particular PFSA.

Theorem 10 ($e$-Synchronization of XPFSA via Projective Composition). Given stationary ergodic QSPs $H_a, H_b$ over alphabets $\Sigma_a, \Sigma_b$, with $A = (Q, \Sigma_a, \delta, \pi)$ being a PFSA encoding $H_a$, and $B^x = (Q^x, \Sigma_a, \delta^x, \pi_{x_a})$ being a XPFSA from $H_a$ to $H_b$, a string $x_0 \in \Sigma_a^*$ is $e$-synchronizing with respect to $B^x$ (in the sense of Definition 24), if $x_0$ is $e$-synchronizing with respect to the PFSA $A \otimes B^x$ (in the sense of Definition 10).

Proof: We note that Lemma 19 implies that for any $x_0 \in \Sigma_a^*$,

$$\max_{x \in \Sigma_a^*} \rho_{x_0}^{H_a, \pi_{x_0}} \geq 1 - e$$

$$\Rightarrow \exists q \in Q_a \left\| E \phi_{x_0}^{H_a, \pi_{x_0}} - \pi_{x_0}(q, \cdot) \right\|_\infty \leq e$$

(145)

Noting that Definition 23 implies:

$$\rho_{x_0}^{H_a, \pi_{x_0}} = \left[ A \otimes B^x \right] q_0$$

(146)

completes the proof.

Thus, to $e$-synchronize the XPFSA $B^x$, we simply need to find an $e$-synchronizing string for the PFSA $A \otimes B^x$ which is a problem that we have already solved (See Lemma 7 and Theorem 5). However,
the definition of the derivative heap (See Definition 13) would need to be suitably generalized (See Definition 27).

However, before we go into XPFSA inference, we note that the above reduction leads us to the following important corollary, which establishes that e-synchronizing strings exist for any \(\epsilon > 0\).

**Corollary 5** (To Theorem 10) Existence of e-Synchronizing Strings for XPFSA. For any \(\epsilon > 0\), stationary ergodic QSPs \(\mathcal{H}_A, \mathcal{H}_B\) over alphabets \(\Sigma_A, \Sigma_B\), and a given XPFSA \(B^*\) from \(\mathcal{H}_A\) to \(\mathcal{H}_B\), there exists a string \(s_0 \in \Sigma_A^*\) that e-synchronizes \(B^*\).

**Proof:** Follows immediately from Theorems 10 and 2. \(\square\)

Before we present our inference algorithm \texttt{xGenESeSS}, we need an effective approach to compute cross-derivatives. First we generalize the count function introduced in Definition 11.

**Definition 25** (Symbolic Cross-Count Function). For strings \(s_A, s_B\) over respective alphabets \(\Sigma_A, \Sigma_B\), the cross-count function \(\#^{A+B}(\cdot)\) counts the number of times a particular substring occurs in \(s_A\), being followed immediately by a symbolic element of string \(s_B\). The count is overlapping, i.e., in strings \(s_A = 000100, s_B = 012212\), we count the number of occurrences of string 00 in \(s_A\), followed immediately by symbol 2 in \(s_B\), as:

\[
\begin{align*}
000100 & \quad 000100 \\
012212 & \quad 012212
\end{align*}
\]

implying \(\#^{A+B}(00, 2) = 2\).

And, then we define an estimator for cross-derivatives using the cross-count function.

**Definition 26** (Cross-derivative Estimator). For strings \(s_A, s_B\) over respective alphabets \(\Sigma_A, \Sigma_B\), the cross-derivative estimator \(\phi^{A+B}(\cdot)\) over \(\Sigma_A^*\) is a non-negative vector summing to unity, with entries defined as:

\[
\forall x \in \Sigma_A^*, \phi^{A+B}(x) = \frac{\#^{A+B}(x, \cdot)}{\sum_{y \in \Sigma_B} \#^{A+B}(y, \cdot)}
\]

And, as before (See Theorem 5), we have the following convergence.

**Lemma 20** (e-Convergence for Cross-derivatives). For stationary ergodic QSPs \(\mathcal{H}_A, \mathcal{H}_B\) over \(\Sigma_A, \Sigma_B\), producing respective strings \(s_A, s_B\), and a given XPFSA \(B^*\) from \(\mathcal{H}_A\) to \(\mathcal{H}_B\), if \(x \in \Sigma_A^*\) is e-synchronizing, then:

\[
\forall \epsilon > 0, \lim_{\|s_A\| + \|s_B\| \to \infty} \|\phi^{A+B}(s_A) - \pi_B(x)\|_\infty \leq \epsilon
\]

**Proof:** Since \(\phi^{A+B}\) is an empirical distribution for \(\phi^{A+B}\), the result follows from Glivenko-Cantelli theorem 39, using the argument of Theorem 5. \(\square\)

In close analogy to PFSA inference described in Section 5, here we seek similar cross-derivatives, and “merges” string arguments at which the derivatives turn out to be similar, i.e. define them to reach the same state in the inferred XPFSA. First we need to generalize the definition of the derivative heap as follows:

**Definition 27** (Cross-Derivative Heap). For stationary ergodic QSPs \(\mathcal{H}_A, \mathcal{H}_B\) over \(\Sigma_A, \Sigma_B\), producing respective strings \(s_A, s_B\), a cross-derivative heap \(\mathcal{D}^{A+B}\) is the set of strings \(\mathcal{D}^{A+B} = \{x \in \Sigma_A^* : x \in \mathcal{L} \subset \Sigma_A^*\}\) calculated for a subset of strings \(L \subset \Sigma_A^*\) as:

\[
\mathcal{D}^{A+B}(L) = \{\phi^{A+B} : x \in \mathcal{L}\}
\]

We note that Lemma 7 and Theorem 4 generalizes immediately:

**Lemma 21** (Cross-derivative Heap Coverage). 1) Define:

\[
\mathcal{D}_{\omega} = \lim_{\|s_A\| + \|s_B\| \to \infty} \mathcal{D}^{A+B}(L)
\]

If \(\omega\) is the convex hull of \(\mathcal{D}_{\omega}\), \(u\) is a vertex of \(\omega\) and \(\pi_{\omega}\) is the output morph the XPFSA from \(\mathcal{H}_A\) to \(\mathcal{H}_B\), then we have:

\[
\exists \epsilon > 0, \text{such that } u = \pi_{\omega}(q, \cdot)
\]

2) For stationary ergodic QSPs \(\mathcal{H}_A, \mathcal{H}_B\) over \(\Sigma_A, \Sigma_B\), producing respective strings \(s_A, s_B\), let \(\mathcal{D}^{A+B}\) be computed as \(\mathcal{L} = \{x \in \Sigma_B \mid \phi^{A+B}\text{ is a vertex of the convex hull of }\mathcal{D}^{A+B}(L)\text{, then we have:}\}

\[
\Pr(x_0 = \text{not e-synchronizing}) \leq e^{-\|s_A\|/p_0}
\]

where \(p_0\) is the probability of encountering \(x_0\) in \(s_A\).

**Proof:** See Lemma 6 and Theorem 4. \(\square\)

**6.1 Implementation Steps For xGenESeSS**

We have two steps in xGenESeSS which infers the strongly connected minimal realization \(B^t = (Q_s, \Sigma, \delta, \pi_{\omega})\):

1) **Identification of e-synchronizing string \(x_0\):** Construct a derivative heap \(\mathcal{D}^{A+B}(L)\) using the observed traces \(s_A, s_B\), (Definition 27), and set \(L = \log_{\|s_A\|} 1/e\). We then identify a vertex of the convex hull for \(\mathcal{D}_{\omega}\) via any standard algorithm for computing the hull [44]. Choose \(x_0\) as the string mapping to this vertex.

2) **Identification of the transition function:** We generate \(\delta\) as follows: For each state \(q\), we associate a string identifier \(x^{q}_D = x^{q}_D\), and a probability distribution \(h^{q}_{\omega}\) on \(\Sigma\), (which is an approximation of the \(\Pi_{\omega}\)-row corresponding to state \(q\)). We extend the structure recursively:

   a) Initialize the set \(Q\) as \(Q = \{q_0\}\), and set \(x^{q}_D = x_0\), \(h^{q}_{\omega} = \phi^{q_{0}}(x_0)\).

   b) For each state \(q \in Q_s\), compute for each symbol \(\sigma \in \Sigma\), find symbolic derivative \(\phi^{q_{0}}(\sigma\cdot)\).

      - If \(\|\phi^{q_{0}}(\sigma\cdot) - h^{q}_{\omega}\|_{\infty} \leq \epsilon\) for some \(q' \in Q_s\), then define \(\delta(q, \sigma) = q'\).

      - If, on the other hand, no such \(q'\) can be found in \(Q_s\), then add a new state \(q'\) to \(Q_s\), and define

        \[
        x^{q'}_D = x^{q}_{D} \cdot \sigma, \quad h^{q'}_{\omega} = \phi^{q_{0}}(\sigma\cdot)
        \]

      - The process terminates when every \(q \in Q_s\) has a target state, for each \(\sigma \in \Sigma\).

   Then, if necessary, we ensure strong connectivity using Tarjan’s algorithm [45].

   - The output morph function \(\pi_{\omega}\) is given by:

     \[
     \forall q \in Q_s, \pi_{\omega}(q, \cdot) = h^{q}_{\omega}
     \]

**6.2 Complexity of xGenESeSS & PAC Learnability**

Asymptotic time complexity for xGenESeSS is essentially identical to that of GenESeSS. We have the following immediate result:

**Theorem 11** (Time Complexity). Assuming the input streams are longer compared to the respective alphabet sizes, the asymptotic runtime complexity of xGenESeSS is:

\[
\mathcal{T} = O\left(\frac{\log\left(|\pi_{\omega}(s_A)| + |s_A|\right)}{\epsilon}\right)
\]

**Proof:** Follows from the argument in Theorem 6 noting that the step corresponding to C1 (See Theorem 5) takes \(O(1/\epsilon |s_A| + |s_A|)\) time, the step corresponding to C2 takes \(O(1/\epsilon |\Sigma_A|)\) time and the step corresponding to C3 takes \(O(|\pi_{\omega}(s_A)| + |s_A|)\) time. \(\square\)

**Lemma 22** (Metric For Cross Probabilistic Automata). For stationary ergodic QSPs \(\mathcal{H}_A, \mathcal{H}_B\) over alphabets \(\Sigma_A, \Sigma_B\), and \(\mathcal{H}_A, \mathcal{H}_B\) over \(\Sigma_A, \Sigma_B\), let \(G_1, G_2\) be XPFAs representing the transition functions from \(\mathcal{H}_A\), \(\mathcal{H}_B\) to \(\mathcal{H}_A, \mathcal{H}_B\) respectively. If \(s_A, s_B, s'_A, s'_B\) are string generated by \(\mathcal{H}_A, \mathcal{H}_B, H'_A, H'_B\) respectively, then:

\[
\delta_{s_A, s_B}(G_1, G_2) = \sup_{x \in \Sigma_A^*} \left\{ \lim_{\|s_A\| + \|s_B\| \to \infty} \|\phi^{A+B}(s_A) - \phi^{A+B}(s'_A)\|_{\infty} \right\}
\]

defines a metric on the space of cross probabilistic automata that represent dependencies from processes over \(\Sigma_A\) to processes over \(\Sigma_B\).
Theorem 12 (PAC-Learnability). The dependency between two ergodic stationary QSPs $\mathcal{H}_1, \mathcal{H}_2$ over respective alphabets $\Sigma_1, \Sigma_2$ with an ergodic, consistent cross-talk map (Definition 7) is learnable by xGenESeSS in the following sense:

If $G$ denotes the true XPFSA, then $\forall \epsilon, \eta > 0$, xGenESeSS learns an estimated XPFSA $G'$ with:

$$Pr(\Theta_{x,y}(G, G') \geq \epsilon) < \eta$$

and the asymptotic runtime is polynomial in $1/\epsilon, |\Sigma_1| + |\Sigma_2|, 1/\eta$.

Additionally, to satisfy the above condition, we need:

$$|\Sigma_1| + |\Sigma_2| = O\left(\frac{1}{\epsilon} C^{0.6} \log \frac{1}{\eta}\right)$$

where $C < \infty$, and $Q$ is the set of states in the inferred XPFSA.

Proof: On account of Theorem 10, the result in Eq. (158) follows from the same argument as in Theorem 9 (using Eq. (152) instead of Eq. (7)). The sample complexity also follows from the same argument, with the modification of including the sum of string lengths arising from Theorem 11.

7 Generation of Causality Networks

The coefficient of causal dependence was introduced in Definition 22 to quantify the reduction in uncertainty of the next symbol in the second stream from observations made in the first. It was clear that this coefficient is asymmetric, in the sense that in general for two ergodic stationary QSPs $\mathcal{H}_1, \mathcal{H}_2$, we have:

$$\gamma^{H_1}_{i,j} \neq \gamma^{H_2}_{i,j}$$

Additionally, the example in Figure 3 demonstrates that the coefficients do indeed capture directional dependence, i.e., the direction of causality flow between two processes. We can extend this idea to a set of interdependent processes; the calculation of the pairwise coefficients would then reveal the possibly intricate flow of causality, leading to what we call the inferred causality network.

Consider the set of $n$ ergodic stationary processes

$$\mathcal{H} = \{H_i : i = 1, \cdots, n\}$$

evolving over respective alphabets $\Sigma_i$, which need not be distinct or have the same cardinalities.

Let the processes possibly depend on each other via cross-talk maps that satisfy the properties set forth in Definition 14. Additionally, assume that the relevant cross-Nerode equivalences have finite indices, implying that there exist XPFSA that encode the inter-process dependencies.

Notation 6 (Set of Processes and Inferred Machines). We introduce some notation to denote the relevant inferred machines.

- $s' \in \Sigma_i^*$ denotes the string generated by the process $H_i$.
- $H'_i$ with $i \neq j$ denotes the XPFSA from process $H_i$ to $H_j$, where $H'_i = (Q'_i, \Sigma_i, \delta_i, \pi_i)$ (162)
- $H'$ denotes the PFSAs encoding the process $H_i$ itself, where $H' = (Q', \Sigma', \delta', \pi')$ (163)
- The coefficient of dependence from $H'_i$ to $H_j$ is denoted $\gamma'$

We introduce the stream-run function, which would simplify the computation of the coefficients of dependence in the sequel.

Definition 28 (Stream-run Function). Given a strongly connected labeled graph $G = (Q, \Sigma, \delta)$ be a strongly connected graph with $Q$ as the set of nodes, such that there is a labeled edge $q_i \rightarrow q_j$ for $q_i, q_j \in Q$ if $\delta(q_i, \sigma) = q_j$, and string $s \in \Sigma^*$, the stream-run function $\rho(G, s)$ is a real-valued vector of length $|Q|$ with

$$\forall i, \rho(G, s)_i \in [0, 1], \text{and } \sum_{i \in Q} \rho(G, s)_i = 1$$

and is computed using Algorithm 1.

Algorithm 1: Stream-run Function

Input: Strongly connected labeled graph $G = (Q, \Sigma, \delta)$, string $s \in \Sigma^*$
Output: $\rho(G, s)$

1. Initialize zero vector $v$ of length $|Q|
2. Choose random node $q_0 \in Q$
3. $q_{current} \leftarrow q_0$
4. $v_q \leftarrow 1$
5. for $i \leftarrow 1$ to $|s|$
6. \hspace{1em} $q_{current} \leftarrow \delta(q_{current}, s_i)$
7. \hspace{1em} if $q_{current} = q_i$ then
8. \hspace{2em} $v_q \leftarrow v_q + 1$
9. \hspace{1em} /* Normalize vector */
10. return $\rho(G, s) \leftarrow v$

Algorithm 2: Efficient Computation of the Coefficient of Dependence

Input: $\epsilon, s', s''$
Output: Estimate $\gamma'$ for $\gamma''$

// Compute XPFSA
1. Compute $H'_i$
2. $r \leftarrow [0 \cdots 0]$
3. Length $= |\Sigma_j|$
4. for $k \leftarrow 1$ to $|s'|$
5. \hspace{1em} $r_t \leftarrow r_t + 1$
6. Compute denominator $\sum_{j \in Q} \log_2(r_k)$
7. $h_0 \leftarrow 0$
8. $u \leftarrow \rho(H', s')$
9. for $k \leftarrow 1$ to $|Q_j|$
10. \hspace{1em} $h_k \leftarrow \sum_{\gamma \in \Gamma_j} h(\gamma)_k$
11. $h_k \leftarrow h_k + u_k h[k]$
12. return $\gamma' \leftarrow h_1$ (165)

We need the following technical result, that establishes the connection between the stream-run function and the projected distribution introduced in Definition 21.

Lemma 23 (Computing Projected Distribution). Let $s \in \Sigma^*$ be generated by an ergodic stationary QSP $H$ with a finite index Nerode equivalence induced by the underlying probability space $(\Sigma^*, B, \mu)$. Let the minimal PFSAs encoding encoding the QSP be $G = (Q, \Sigma, \delta, \pi)$. Additionally, let $G' = (Q', \Sigma', \delta')$ be a strongly connected graph with $Q'$ as the set of nodes, such that there is a labeled edge $q_i \rightarrow q_j$ for $q_i, q_j \in Q'$ if $\delta'(q_i, \sigma) = q_j$. Then, we have:

$$\lim_{|s| \to \infty} \rho(G', s) =_{\text{a.s.}} G \otimes G' \otimes G'$$

Proof: Since $H$ is ergodic and stationary, and $G \otimes G'$ is a non-minimal but strongly connected realization, it follows that $\rho(G \otimes G', s)$ converges almost surely to the unique stationary distribution $\phi'$ on the state space of $G \otimes G'$. Consider the paths through $G \otimes G'$ and through $G'$ for the string $s$ in the course of computing the respective stream-run functions $\rho(G \otimes G', s)$ and $\rho(G', s)$. Noting that the count of the visits $v(s')$ for the states $(q, q')$ in $G \otimes G'$ relates to the count of visits $v_s$ for state $q'$ in $G'$ as:

$$v_{s'} = \sum_{q \in Q} v(s'q)$$

Let $Q' \subseteq Q$ and $Q' \subseteq Q'$ be the sets of states.

We then have:

$$\lim_{|s| \to \infty} \rho(G', s) =_{\text{a.s.}} G \otimes G' \otimes G'$$
We conclude that:

\[ \rho(G', s) \xrightarrow{\infty} u \]

where the vector \( u \) satisfies:

\[ u = \sum_{q \in Q} \phi_0^{q} \tau_q(s_{q}) \]  

(168)

Recalling the Definition 22 completes the proof.

Based on Lemma 23 Algorithm 2 computes the coefficient of dependence avoiding explicit computation of the projective composition. Next, we establish correctness and complexity of the algorithm.

**Theorem 13 (Error Bound & Complexity of Algorithm 2).** We have:

1. Given the parameter \( \epsilon \) for XPFLSA inference, the absolute error in the estimated coefficient \( \gamma_i \) (See Algorithm 2) satisfies:

\[ \forall \epsilon \in (0, 1/2], \lim_{|y_i - \gamma_i| \to 0} \frac{1}{h(\theta)} \left( \log_2 \frac{\Sigma | - 1 - \epsilon}{\epsilon} + (1 - \epsilon) \log_2 \frac{1}{1 - \epsilon} \right) \]  

(169)

where \( \sigma_i \) occurs with probability \( \theta_i \) in process \( H_i \).

2. Assuming \( |Q_i| \ll 1 \), and \( |r| = |q|, \) the asymptotic run-time complexity of Algorithm 2 is \( O \left( \frac{1}{h(\theta)} |q| |\Sigma| \right) \), i.e., the same as for computing only the XPFLSA \( H_i' \).

**Proof:** As before, we assume the streams \( s', s'' \) to be generated by the processes \( H_i, H_i' \) respectively.

Statement 1): The denominator of \( \gamma_i \) is given by \( h(s_i') \) (Lemma 16), which is the vector of probabilities with which different symbols appear in \( s' \). It follows from ergodicity, that \( r \) in lines 3-5 in Algorithm 2 converges almost surely to the denominator. Lemma 23 guarantees that \( u \) (lines 8-11) converges almost surely to \( \|H' \otimes H_i'\|_{HF_i} \).

Assume that the error in infinity norm between the inferred and actual vectors for any row of \( \Pi_i \) is bounded above by some \( \epsilon \in (0, 1/2) \) almost surely. We refer to this as Assumption A.

Now, let \( u^0 = \|H' \otimes H_i'\|_{HF_i} \), and for all \( q_i \in Q_i \) the true probability vector corresponding to the inferred \( \widehat \gamma_i(q_i, \cdot) \) be \( \epsilon(q_i, \cdot) \). Also, let:

\[ w^0 = \left\{ \left( h(q_i, \cdot) \right), \cdot \right\}, w = \left\{ \left( \widehat \gamma_i(q_i, \cdot) \right), \cdot \right\} \]  

(170)

Then, we have:

\[ |y_i - \gamma_i| \leq \frac{\left\langle u^0, w^0 \right\rangle - \left\langle u, w^0 \right\rangle + \left\langle u, w^0 \right\rangle - \left\langle u, w \right\rangle}{h(r)} \]  

(171)

\[ \leq \frac{\left\langle u^0 - u, w^0 \right\rangle + \left\langle u, w^0 - w \right\rangle}{h(r)} \]  

(172)

\[ \leq \frac{\left\langle u^0 - u, w^0 \right\rangle}{h(r)} + \frac{\left\langle u, w^0 - w \right\rangle}{h(r)} \]  

(173)

We note that \( u \xrightarrow{\epsilon} u^0 \), and \( h(r) \xrightarrow{\epsilon} h(\theta) \), and by Assumption A:

\[ \forall q_i \in Q_i, \|e(q_i, \cdot) - \widehat \gamma_i(q_i, \cdot)\|_{HF_i} \leq \epsilon \]  

(174)

which implies (See 21, Lemma 7) that if \( \epsilon \leq 1/2 \), then we have:

\[ \forall q_i \in Q_i, \|w_i^0 - w_i\|_{HF_i} \leq \epsilon \log_2 \frac{\Sigma |}{\epsilon} + (1 - \epsilon) \log_2 \frac{1}{1 - \epsilon} \]  

(175)

Hence, we conclude, that given Assumption A, we have:

\[ \lim_{|y_i - \gamma_i| \to 0} \frac{1}{h(\theta)} \left( \log_2 \frac{\Sigma |}{\epsilon} + (1 - \epsilon) \log_2 \frac{1}{1 - \epsilon} \right) \]  

(176)

Now, Definition 22 implies that Assumption A is equivalent to:

\[ \Theta_{r, \Sigma}(H_i', H_i') \leq \epsilon \]  

(177)

where \( H_i', H_i' \) are respectively the true and estimated XPFLSAs for the cross-dependency from the process \( H_i \) to the process \( H_i' \). It follows from Theorem 12 that:

\[ \forall \epsilon \in (0, 1/2), \]  

(180)

**Algorithm 3: Prediction of Next-symbol Distribution From Cross-talk**

**Input:** \( \epsilon, s', s'', \cdot \)

**Output:** Predicted next-symbol distribution \( r' \)

1. Compute \( H' = \left(Q_i, \Sigma, \delta_t, \Pi_{HF_i} \right) \) using \( s', \epsilon \)
2. Compute \( H'_\Pi = \left(Q_{HF_i}, \Sigma, \delta_t, \Pi_{HF_i} \right) \) using \( s', s'', \epsilon \)
3. \( G \rightarrow H' \otimes H'_\Pi \)
4. Compute stationary distribution \( s'_G \)
5. \textbf{foreach} \( \sigma \in \Sigma \) \textbf{do}
6. \quad \textbf{Compute} \( \Pi_{HF_i}^{s'} \)
7. \quad \textbf{for} \( k \rightarrow 1 \rightarrow |s_i| \) \textbf{do}
8. \quad \quad \textbf{Compute} \( \Pi_{HF_i}^{s'} \)
9. \quad \quad \textbf{return} \( r' \rightarrow \gamma_i' \Pi_{HF_i}^{s'} \)

(178)

which establishes Statement 1). Statement 2) follows immediately from Theorem 11.

**Remark 4.** We note that \( \frac{1}{h(\theta)} > 0 \) implies:

\[ \lim_{|y_i - \gamma_i| \to 0} \frac{\epsilon \log_2 \frac{\Sigma |}{\epsilon} + (1 - \epsilon) \log_2 \frac{1}{1 - \epsilon}}{1 - \epsilon} = 0 \]  

(179)

i.e., the bound established in Theorem 13 is small for small values of \( \epsilon \). It is important to consider the implication of the factor \( 1/h(\theta) \). In particular, for the bound to be finite, we must assume that the process \( H_i \) does not only produce a single repeated symbol, since in that case \( h(\theta) = 0 \). Also, if the process \( H_i \) has a single symbol occurring with an overwhelmingly high probability, then \( h(\theta) \) would be small, which would then imply that a longer \( s' \) is required. This observation is relevant in applications with relatively rare events; e.g., networks of spiking neurons, or when attempting to construct causality networks from global seismic data.

### 7.1 Prediction Using Crossed Probabilistic Automata

Inferred cross-talk between data streams may be exploited for predicting the future evolution of the processes under consideration. We use the same notation as before. However, in addition to the set of \( n \) ergodic processes \( \mathcal{H} = \{H' : i = 1, \ldots, n\} \), we consider an additional process \( H_n \), evolving over the alphabet \( \Sigma_n \) (with the same standard assumptions). We are interested in predicting the future evolution of \( H_n \).

**Notation 7 (Additional Notation).** \( \bullet \) In accordance to the naming scheme described in the previous section (See Notation 2), the XPFLSA from \( H_i \) to \( H_n \) is denoted \( H_{n}^i = \left(Q_{HF_i}, \Sigma, \delta_t, \Pi_{HF_i} \right) \).

\( \bullet \) \( s_n \in \Sigma_n \) is the string observed in the process \( H_n \).

\( \bullet \) In addition to the strings \( s' \) (See Notation 2), we observe relatively short strings \( x' \in \Sigma_i, i = 1, \ldots, n \) respectively in the \( n \) processes \( H_i \), which represent the immediate histories.

\( \bullet \) In particular, we use \( s \), for the stream from process \( H_i \) when we are inferring machines, and use \( x' \) when we need a short history for state localization (explained in the sequel).

\( \bullet \) \( r', i = 1, \ldots, n \) denotes the expected next-symbol distribution in process \( H_n \) computed using the cross-talk or dependency from \( H_i \) to \( H_n \) (assuming that the immediate history observed in the former is \( s' \)). Thus, we have:

\[ \forall H_i \in \mathcal{H}, \left\{ \forall k, r_i' \in [0, 1], \right\} \sum_{i = 1}^{n} r_i' = 1 \]  

(180)
Lemma 24. Let $G \in H \circlearrowleft H$, and let $\varphi^t_i$ be the realized distribution over the states of PFSA $G = (Q_m, \Sigma_i, \vartheta_{is}, \omega_i)$, given the occurrence of string $x^t ∈ Σ^t_i$ beginning with the stationary distribution $\varphi^0_i$. Then:

$$\tau^t = \varphi^t_i \pi_B$$  \hspace{1cm} (181)

where $\varphi^t_i$ is assumed to be a row vector.

Proof: We note that Lemma 19 tells us:

$$\tau^t = \mathbf{E} \varphi^t_i \pi_B = \varphi^t_i \pi_B$$  \hspace{1cm} (182)

The result then follows from Definition 8 (Canonical Representation) and Definition 23 (Induced Cross-Distribution).

Algorithm 3 illustrates the pseudo-code for computing $\tau^t$.

7.1.1 Fusion of Individual Predictions:

The problem of fusing the predictions $\tau^t$ for the processes in $H$ to yield the “best” prediction $\overline{\tau}$, only admits a heuristic solution (at least with no further information). One approach to carry out this fusion is simply to take the weighted average of the predicted distributions, with the weights chosen to be normalized coefficients of dependence:

$$\text{Prediction Fusion:} \quad \overline{\tau} = \frac{1}{T} \sum_{t=1}^{T} \left( \frac{\gamma^t}{\sum_{t} \gamma^t} \right) \tau^t$$  \hspace{1cm} (183)

This combination strategy assigns zero weight to processes for which the corresponding coefficient of dependence is null.

8 Application To Internet Search Trends

Google Trends (http://www.google.com/trends/) provides a convenient API to download time series of weekly search frequencies for any given keyword. The time series’ are normalized between [0, 100], and corresponding to a particular keyword, each integer-valued entry of the data series indicates the weekly sum-total of normalized worldwide queries submitted to the google website. Data is typically available from the first week of January, 2004. Thus, at the time of writing this paper, each of these search-trend data series are ~ 548 entries long. We selected a small sample of keywords, typically ones that are strongly “charged” in a political or social context. The set of keywords are shown in Table 1.

A. Strongly Correlated Search-keywords With No Causal Relationship

| (1) climate change | (2) constitution | (3) drugs | (4) economy |
|-------------------|-----------------|-----------|------------|
| (5) education     | (6) environment | (7) freedom | (8) global warming |
| (9) god           | (10) government | (11) guns | (12) healthcare |
| (13) immigration  | (14) industry   | (15) literature | (16) music |
| (17) nuclear      | (18) nuclear weapons | (19) oil | (20) peace |
| (21) religion     | (22) science    | (23) tax  | (24) terrorism |
| (25) war          | (26) wealth     |

B. Causally Related Search-keywords

C. Coefficients of causal dependence ($\gamma$) Between Keywords

Fig. 7. Illustration that high statistical correlation does not signal a high degree of causal dependency. Plate A: Strongly positively correlated $\gamma = 0.96$ search-frequency data for keywords “education”, “environment”. Plate B: Positively correlated $\gamma = 0.75$ search-frequency data for keywords “economy”, “government”. Plate C shows that the data in plate A have little causal dependence in either direction, while those in plate B have a directional causal dependence. The weights on the arcs in plate C are values for the inferred coefficient of causal dependence $\gamma$. As per definition 7, “education” 0.199691 “government” implies: 1 bit of information from the search-frequency data for “education” reduces the uncertainty in the immediate future of the data for “government” by 0.199691 bits.

To “education” has little or no causal dependence on the data for “environment”. While, despite having a lower correlation, search-frequency for “economy” and “government” seem to be strongly causally related, in one direction. Based on the discussion in Section 8 this is entirely possible; while the plots in plate A of Figure 7 are seemingly very close (which leads to the strong statistical correlation), this has nothing to do with causality - what matters is if one data series carries unique information that can improve prediction of the other.

Note here an interesting consequence from Granger’s notion of causality: Two identical data series necessarily have no causal relationship; if series’ $X$ and $Y$ are identical, i.e., $X_t = Y_t, \forall t$, then neither can improve the prediction of the other.

The full causality network for the keywords in Table 1 is shown in Figure 8. We used a binary quantization to map each integer valued...
9 Conclusion

We presented a new non-parametric approach to test for the existence of the degree of causal dependence between ergodic stationary weakly dependent symbol sources. In addition, the notion of generative cross-models is made precise, and it is shown that crossed probabilistic automata are sufficient to represent a fairly broad class of direction-specific causal dependencies; and that they may be inferred efficiently from data. Efficient inference of the coefficient of causal dependence, defined here, gives us the ability to investigate the network of causality flows between data sources. It is hoped that the theoretical development presented here will open the door to understanding hidden mechanisms in diverse data-intensive fields of scientific inquiry.

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Fig. 8. Full causality network computed with weekly search-frequency data corresponding to the keywords tabulated in Table I from Google Trends API. The size of the nodes, as well as the degree of “redness” is indicative of the weighted degree. The thickness of the arcs are indicative of the coefficient of causal dependence (γ). “religion” seems to have a particularly high degree.

data series to a symbol stream; with symbol “0” indicating a drop in the search frequency from the previous week, and a “1” indicating identical or increased frequency. The size of the nodes, as well as the degree to which they are colored red, indicate the weighted degree of the graph. It appears that “religion” has a particularly high degree.
