A New View of Predictive State Methods for Dynamical System Learning

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Abstract
Recently there has been substantial interest in predictive state methods for learning dynamical systems: these algorithms are popular since they often offer a good tradeoff between computational speed and statistical efficiency. Despite their desirable properties, though, predictive state methods can sometimes be difficult to use in practice. E.g., in contrast to the rich literature on supervised learning methods, which allows us to choose from an extensive menu of models and algorithms to suit the prior beliefs we have about properties of the function to be learned, predictive state dynamical system learning methods are comparatively inflexible: it is as if we were restricted to use only linear regression instead of being allowed to choose decision trees, nonparametric regression, or the lasso. To address this problem, we propose a new view of predictive state methods in terms of instrumental-variable regression. This view allows us to construct a wide variety of dynamical system learners simply by swapping in different supervised learning methods. We demonstrate the effectiveness of our proposed methods by experimenting with non-linear regression to learn a hidden Markov model, showing that the resulting algorithm outperforms its linear counterpart; the correctness of this algorithm follows directly from our general analysis.

1 Introduction
Recently, there has been substantial interest in a new class of algorithms for learning dynamical systems. These algorithms combine several key intuitions, of which two are important to the current discussion.
First is the idea of **predictive state**: we can replace a belief about a latent variable $S$ by the prediction of some observable variables $X$ that depend on $S$. That is, on observing some evidence $E$ about $S$, we could calculate the belief $P(S \mid E)$. But, as long as the function $f(S) = \mathbb{E}(X \mid S)$ is sufficiently rich (e.g., for discrete $X$ and $S$ represented by one-hot encodings, invertible), it is equivalent to calculate $\mathbb{E}(X \mid E)$ directly: we could recover $P(S \mid E)$ by inverting $f$, but in many cases we don’t need to do so.

Second is the **method of moments**: for a dynamical system model with parameters $\theta$, it is often intractable to solve the maximum likelihood problem

$$\max_{\theta} \ln P(\text{observations} \mid \theta)$$

But, we can sometimes find a statistic $T$ such that the expectation of $T$ is a simple, invertible function of $\theta$: $\mathbb{E}_{\theta}(T) = g(\theta)$. In this case, we can replace the expectation $\mathbb{E}_{\theta}(T)$ with the empirical average $\hat{T} = \frac{1}{N} \sum_{i=1}^{N} T_i$. (Here $T_i$ is the value of our statistic for the $i$th of a set of $N$ observations.) We can then define an estimator $\hat{\theta}$ as

$$\hat{\theta} = g^{-1}(\hat{T})$$

and seek an efficient algorithm for solving the inverse problem (1). The trick to designing a good method of moments algorithm is to discover a statistic $T$ such that problem (1) is well-conditioned and efficiently solvable. One of the main tools that algorithm designers use for this purpose is to expand the class of models considered, thereby removing difficult constraints from (1): for example, instead of learning a hidden Markov model (HMM), we can expand the model class to include all observable operator models (OOMs) [14].

For brevity, we will call methods that use the above intuitions **predictive state methods**. Predictive state methods are popular for dynamical system learning because they often offer a good tradeoff between computational speed and statistical efficiency.

However, there are also some important difficulties with these methods. One is that it can be hard for predictive state methods to take advantage of prior knowledge about the structure or parameters of a dynamical system: for example, expanding from HMMs to OOMs removes our ability to directly refer to the conditional probability distribution of observations given states, a common place to incorporate structure. Another is that deriving, analyzing, and implementing new predictive state methods can require substantial expertise: it can be difficult to discover an appropriate statistic $T$, accumulate its empirical average $\hat{T}$ efficiently,
and track how estimation errors in $\hat{T}$ propagate through the inverse problem (1) to affect $\hat{\theta}$.

We address both of these problems with a new view of predictive state methods for dynamical system learning. In this view, a dynamical system learning problem is reduced to a sequence of supervised learning problems. So, we can directly apply the rich literature on supervised learning methods to incorporate many types of prior knowledge about problem structure. We give a general convergence rate analysis that allows a high degree of flexibility in designing estimators. And finally, implementing a new estimator becomes as simple as rearranging our data and calling the appropriate supervised learning subroutines.

Our new view is based on instrumental variable regression [18, 22]. Instrumental variable regression is a well-known technique to compensate for certain types of observation noise in a linear regression problem; it can let us recover regression coefficients accurately where ordinary regression would yield biased estimates. The connection between predictive state learning and linear instrumental variable regression has been noted before, e.g., in [4]. We propose a generalization of the linear two stage ordinary least squares procedure [22], give error bounds for this generalization, and formulate dynamical systems learning as an instance of this regression technique.

More specifically, our contribution is to show that we can use much-more-general supervised learning algorithms in place of linear regression, and still get a meaningful theoretical analysis. In more detail: (1) we point out that we can equally well use any well-behaved supervised learning algorithm in place of linear regression in the first stage of instrumental-variable regression; (2) for the second stage of instrumental-variable regression, we generalize ordinary linear regression to its RKHS counterpart; (3) we analyze the resulting combination, and show that we get convergence to the correct answer, with a rate that depends on how quickly the individual supervised learners converge.

In the remainder of the paper, we first describe how to use instrumental-variable regression to learn a dynamical system (Sec. 2). We then provide theoretical guarantees for the two-stage instrumental-variable regression technique with non-linearity (Sec. 4). Finally, we give an example of how our techniques let us rapidly design enhanced predictive state methods for dynamical systems by encoding modeling assumptions (Sec. 5): we show that replacing linear regression steps in the spectral HMM learning algorithm with a non-linear regression with fewer parameters results in better prediction performance. The correctness of the resulting algorithm follows immediately from our general analysis.
2 Instrumental Regression for Dynamical Systems

We consider a dynamical system of the form in Fig. 1: a sequence of observations \( o_t \in \mathcal{O} \) explained by latent states \( s_t \in \mathcal{S} \) connected in a chain. A key question we need to solve in order be able to perform inference in the dynamical system is how to recursively update our belief about state: given a belief about \( s_t \) and a new observation \( o_{t+1} \), compute a belief about \( s_{t+1} \). This is referred to as filtering. Another inference task is prediction: predicting an observation \( o_{t+k} \) given our belief about the current state \( s_t \). This involves computing a belief about future state \( s_{t+1} \) given our belief about \( s_t \).

If \( s_t \) and \( o_t \) have small, discrete ranges, the predictive state algorithm for learning a dynamical system is well known: see, e.g., [6, 3]. In fact, it is also known that we can interpret this algorithm as linear instrumental-variable regression [4]. Our proposed framework generalizes that direction by reducing dynamical system learning to solving three supervised learning problems, with the additional ability to incorporate arbitrary non-linear regression models in two of these problems.

The first step to formulate dynamical system learning as a supervised learning problem is to use an observable (predictive state) representation by replacing our belief about \( s_t \) with a predictive state: pick a statistic \( \psi_t = \psi(o_{t:t+k-1}) \) of a window of future observations \( o_{t+1:t+k} \), and instead of tracking our belief \( \mathbb{P}(s_t \mid o_{1:t-1}) \), track the predictive state \( \mathbb{E}[\psi_t \mid o_{1:t-1}] \). (The dimension of \( \psi \) must be at least as high as the number of discrete latent states.) We will use \( Q_{t\mid t-k} \) to denote \( \mathbb{E}[\psi_t \mid o_{t:t-k}] \) and hence our predictive predictive state is denoted by \( Q_t \equiv Q_{t\mid t-1} \). We assume that the system is \( k \)-observable and hence latent states are distinguishable by the distribution of a window of \( k \) future observations\(^1\) [25].

Second, we formulate a statistic \( \xi_t = \xi(o_{t:t+k}) \) over extended future observations \( o_{t:t+k} \) with conditional expectation \( P_t = \mathbb{E}[\xi_t \mid o_{1:t-1}] \) such that \( Q_{t+1\mid t-1} \) and \( Q_{t+1} \) (i.e. our belief about the shifted future \( o_{t+1:t+k} \)) can be inferred from \( P_t \) and \( o_t \).

\(^1\)In principle, the statistics can depend on the entire future. The restriction to a window of observations simplifies the notation and is commonly used in practice.
Learning a dynamical system then amounts to learning an operator $W$ that satisfies the moment condition:

$$P_t = WQ_t \quad \forall t \quad (2)$$

Filtering and prediction then correspond to inferring $Q_{t+1}$ and $Q_{t+1|t-1}$ respectively from $P_t$. We assume that $W$ is a linear operator. Unfortunately, we do not observe $Q_t$ or $P_t$ but noisy versions thereof. Moreover, due to the overlap between observation windows, the noise terms on $\psi_t$ and $\xi_t$ are correlated. This noise correlation means that naive linear regression (using samples of $\psi_t$ and $\xi_t$) will give a biased estimate of the dependence between $Q_t$ and $P_t$.

To counteract this bias, we employ instrumental regression [18, 22]. Instrumental regression uses instrumental variables that are correlated with the input $Q_t$ but not with the noise $\epsilon_{t:t+k}$. This property provides a criterion to denoise the inputs and outputs of the original regression problem: we remove that part of the input/output that is not correlated with the instrumental variables. Since past observations $o_{1:t-1}$ do not overlap with future or extended future windows, they are not correlated with the noise $\epsilon_{t:t+k+1}$. Therefore, we can use history features $h_t \equiv h(o_{1:t-1})$ as instrumental variables.

In more detail, by taking the expectation of (2) over $h_t$ we obtain an instrument-based moment condition

$$\mathbb{E}[P_t \mid h_t] = \mathbb{E}[WQ_t \mid h_t]$$
$$\mathbb{E}[\mathbb{E}[\xi_t \mid o_{1:t-1}] \mid h_t] = W\mathbb{E}[\mathbb{E}[\psi_t \mid o_{1:t-1}] \mid h_t]$$
$$\mathbb{E}[\xi_t \mid h_t] = W\mathbb{E}[\psi_t \mid h_t] \quad (3)$$

Assuming that there are enough independent dimensions in $h_t$ that are correlated with $Q_t$, we maintain the rank of the moment condition when moving from (2) to (3), and we can recover $W$ by least squares if we can compute $\mathbb{E}[\psi_t \mid h_t]$ and $\mathbb{E}[\xi_t \mid h_t]$ for sufficiently many examples $t$.

In summary, learning and inference of a dynamical system through instrumental regression can be described as follows:

- **Model Specification**: Pick features of history $h_t = h(o_{1:t-1})$, future $\psi_t = \psi(o_{t:t+k-1})$ and extended future $\xi_t = \xi(o_{t:t+k})$. $\psi_t$ must be a sufficient statistic for $\mathbb{P}(o_{t:t+k-1} \mid o_{1:t-1})$. $\xi_t$ must satisfy

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2Note that, similar to [16], $P_t$ is a deterministic function of $Q_t$ and hence this condition has a unique solution if we observe sufficient examples of $P_t$ and $Q_t$. 

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\[ E[\psi_{t+1} | o_{1:t-1}] = f_{\text{predict}}(E[\xi_t | o_{1:t-1}]) \] for a known function \( f_{\text{predict}} \).
\[ E[\psi_{t+1} | o_{1:t}] = f_{\text{filter}}(E[\xi_t | o_{1:t-1}, o_t]) \] for a known function \( f_{\text{filter}} \).

- **S1A (Stage 1A) Regression**: Learn a (possibly non-linear) regression model to estimate \( \bar{\psi}_t \equiv E[\psi_t | h_t] \). The training data for this model are \((h_t, \psi_t)\) across time steps \( t \).

- **S1B Regression**: Learn a (possibly non-linear) regression model to estimate \( \bar{\xi}_t \equiv E[\xi_t | h_t] \). The training data for this model are \((h_t, \xi_t)\) across time steps \( t \).

- **S2 Regression**: Use the feature expectations estimated in the previous two steps to train a model to predict \( \bar{\xi}_t = W \bar{\psi}_t \), where \( W \) is a linear operator. The training data for this model are estimates of \((\bar{\psi}_t, \bar{\xi}_t)\) across time steps \( t \) obtained from S1 steps.

- **Initial State Estimation**: Estimate an initial state \( Q_1 = E[\psi_1] \) by averaging \( \psi_1 \) across several example realizations of our time series.\(^4\)

- **Inference**: Starting from the initial state \( Q_1 \), we can maintain the belief state \( Q_t \equiv E[\psi_t | o_{1:t-1}] \) through filtering: given \( Q_t \) we compute \( P_t \equiv E[\xi_t | o_{1:t-1}] = WQ_t \). Then, given the observation \( o_t \), we can compute \( Q_{t+1} = f_{\text{filter}}(P_t, o_t) \). Or, in the absence of \( o_t \), we can predict the next state \( Q_{t+1|t-1} = f_{\text{predict}}(P_t) \). Finally, by definition, the belief state \( Q_t \) is sufficient to predict \( \mathbb{P}(o_{t:t+k-1} : o_{1:t-1}) \).

The process of learning and inference is depicted in Figure 2. Modeling assumptions are reflected in the choice of the statistics \( \psi, \xi \) and \( h \) as well as the regression models in stages S1A and S1B. In the supplementary material we show that, with linear S1 models and certain choices of statistics, we can recover existing spectral algorithms for dynamical systems learning. The two stage framework not only provides a unifying view of some of the successful dynamical systems learning algorithms but also paves the way for extending them in a theoretically justified manner, as we demonstrate in the experiments.

\(^3\)Our bounds assume that the training time steps \( t \) are sufficiently spaced for the underlying process to mix, but in practice, the error will only get smaller if we consider all time steps \( t \).

\(^4\)This is the only step that needs multiple realizations of our time series. If only a single long realization is available, we need additional assumptions to be able to estimate an initial state; for example, if we assume stationarity, we can set the initial state to be the empirical average vector of future features, \( \frac{1}{T} \sum_{t=1}^{T} \psi_t \).
Figure 2: Learning and applying a dynamical system using instrumental regression. S1 regression is trained to provide data to train S2 regression. At test time, starting from an initial belief state $Q_0$, we alternate between S2 regression and filtering/prediction.

3 Related Work

This work extends predictive state learning algorithms for dynamical systems, which include spectral algorithms for Kalman filters [2], Hidden Markov Models [10, 19] and Predictive State Representations (PSRs) [6, 3] as well as infinite-dimensional variants such as the Hilbert space embedding of hidden Markov models (HSE-HMM) [20] and predictive state representations (HSE-PSR) [5].

One common aspect in all these models is that they exploit the covariance structure between future and past observation sequences to obtain an unbiased observable state representation. Indeed, many of these algorithms can be reformulated as a two-stage linear instrumental regression. Boots and Gordon [4] note the connection between the HSE-HMM and instrumental variables, which is manifested in the use of kernel SVD of a future-past covariance operator to identify the latent state space. We use this connection to build a general framework for dynamical system learning where the state-space can be identified using supervised learning methods, including non-linear ones.

Reducing dynamical systems learning to supervised learning dates back to auto-regressive models [17], where the state of the system is assumed to be fully determined by the previous $k$ observations. Our aim is to use supervised learn-
ing methods to learn latent state models from observation sequences. This bears similarity to Langford et al.’s sufficient posterior representation (SPR) [16], which encodes the state by the sufficient statistics of the conditional distribution of the next observation and represents system dynamics by three vector-valued functions that are estimated using supervised learning approaches. While SPR allows all of these functions to be non-linear, there are some advantages that distinguish our work. First, while SPR is limited to 1-step observable systems (where the distribution over the next observation uniquely determines the state), our framework can seamlessly handle $k$-step observable systems by choosing a large enough (or even unbounded) window size. The use of instrumental variables ensures that correlated noise on overlapping windows does not bias our estimates of the system parameters. Secondly, SPR involves a rather complicated training procedure, involving multiple iterations of model refinement and model averaging, whereas our framework only requires solving three regression problems in sequence. Finally, the theoretical analysis of [16] only establishes the consistency of SPR learning assuming that all regression steps are solved perfectly. Our work, on the other hand, establishes convergence rates based on the performance of S1 regression.

4 Theoretical Analysis

In this section we present our main theoretical result: consistency and a convergence rate bound for two-stage instrumental regression, under the assumption that S1 predictions converge to the true conditional expectations at an appropriate rate, regardless of the functional form of the S1 regressors.

We assume we are given i.i.d. triplets $(x_t, y_t, z_t)$, where $x_t \in \mathcal{X}$, $y_t \in \mathcal{Y}$ and $z_t \in \mathcal{Z}$ denote input, output and instrumental variables respectively. (As mentioned above, we can equally well use correlated samples, as would result from successive time steps of a time series; our convergence rates will then include a factor that depends on the mixing rate of the underlying dynamical system.)

For generality, we assume that $\mathcal{X}$, $\mathcal{Y}$ and $\mathcal{Z}$ are reproducing kernel Hilbert spaces (RKHS) of possibly infinite dimension, and that the operator $\hat{W}$ is estimated through (kernel) ridge regression

$$\hat{W}_\lambda = \left( \sum_{t=1}^{T} y_t \otimes x_t \right) \left( \sum_{t=1}^{T} x_t \otimes x_t + \lambda I_\mathcal{X} \right)^{-1}$$

where $\otimes$ denotes tensor product and $\lambda > 0$ is a regularization parameter that ensures the invertibility of the estimated covariance. $\lambda$ can be 0 in finite dimensional
cases where we have an invertible covariance matrix. The RKHS view is useful when the future statistics are represented in terms of kernels—for example, if they are kernel mean maps of the distribution of future observations, a case that is closely related to the HSE-HMM [20] and HSE-PSR [5] models.

Let \( \bar{x}_t \) and \( \bar{y}_t \) denote \( E[ x_t | z_t ] \) and \( E[ y_t | z_t ] \). Also let \( \hat{x}_t \) and \( \hat{y}_t \) denote \( \hat{E}[ x_t | z_t ] \) and \( \hat{E}[ y_t | z_t ] \), as estimated by the S1A and S1B regression steps. We assume that \( \bar{x}_t, \bar{y}_t \in \mathcal{X} \) and \( \bar{y}_t, \bar{y}_t \in \mathcal{Y} \). Let \( \Sigma_{\bar{x}\bar{x}} \in \mathcal{X} \otimes \mathcal{X} \) and \( \Sigma_{\bar{y}\bar{y}} \in \mathcal{Y} \otimes \mathcal{Y} \) denote the (uncentered) covariance operators of the distributions of \( \bar{x} \) and \( \bar{y} \) respectively: that is,

\[
\Sigma_{\bar{x}\bar{x}} = E[ \bar{x} \otimes \bar{x} ] \quad \Sigma_{\bar{y}\bar{y}} = E[ \bar{y} \otimes \bar{y} ]
\]

Before we state our main theorem we need to quantify the quality of S1 regressions in a way that is independent of the functional form that we assume in S1.

**Definition 1 (S1 Regression Bound).** For a given \( \delta > 0 \) and \( N \in \mathbb{N}^+ \), we define the S1 regression bound \( \eta_{\delta,N} > 0 \) to be a number satisfying the condition that, with probability at least \( (1 - \delta/2) \), the following holds for all \( 1 \leq t \leq N \):

\[
\| \hat{x}_t - \bar{x}_t \|_\mathcal{X} < \eta_{\delta,N} \\
\| \hat{y}_t - \bar{y}_t \|_\mathcal{Y} < \eta_{\delta,N}
\]

As long as, for each fixed \( \delta \),

\[
\lim_{N \to \infty} \eta_{\delta,N} = 0,
\]

our results show that the two stage estimator is consistent:

**Theorem 2.** Assume that \( \| \bar{x} \|_\mathcal{X}, \| \bar{x} \|_\mathcal{Y} < c < \infty \) almost surely. Let \( \eta_{\delta,N} \) be as defined in Definition 1 and assume it satisfies (5). Assume \( W \) is a Hilbert-Schmidt operator, let \( \hat{W}_\lambda \) be as defined in (4), and let \( \hat{R}(\Sigma_{\bar{x}\bar{x}}) \) denote the closure of the range of \( \Sigma_{\bar{x}\bar{x}} \). Then the following statement holds with probability at least \( 1 - \delta \)
for each $x_{\text{test}} \in \mathcal{R}(\Sigma_{x\bar{x}})$ s.t. $\|x_{\text{test}}\|_{X} \leq 1$.

$$\gamma_{\delta,N} \equiv \|\hat{W}_{\lambda}x_{\text{test}} - Wx_{\text{test}}\|_{Y} = O \left( \eta_{\delta,N} \left( \frac{1}{\lambda} + \sqrt{\frac{\log(1/\delta)}{N}} \right) \right)$$

$$+ O \left( \frac{\log(1/\delta)}{\sqrt{N}} \left( \frac{1}{\lambda} + \frac{1}{\lambda^2} \right) \right)$$

$$+ O \left( \sqrt{\lambda} \right)$$

Theorem 2 gives a generic error bound on S2 regression in terms of S1 regression performance. We defer the proof, as well as finite sample analysis, to the supplementary material. The main insight from the theorem is that the error in estimating the parameter $W$ is the sum of three contributions: the first term captures the error in the S1 regressions. The second term captures the effect of estimating the covariance operators from finite data, assuming S1 regression is exact. Finally, the third term captures the effect of regularization assuming covariance estimates are exact. It can be shown that, if $X$ and $Y$ are finite dimensional, $\Sigma_{x\bar{x}}$ spans $X$ and we use least squares to estimate $W$ (i.e. $\lambda = 0$), then the first and last terms will vanish, and $\lambda$ in the middle two terms will be replaced by $\lambda_{x,\text{min}}$, the minimum eigenvalue of $\Sigma_{x\bar{x}}$.

For completeness, the following propositions provide concrete examples of S1 regression bounds $\eta_{\delta,N}$ for practical regression models.

**Proposition 3.** Assume $X \equiv \mathbb{R}^{d_{x}}, \mathbb{R}^{d_{y}}, \mathbb{R}^{d_{z}}$ for some $d_{x}, d_{y}, d_{z} < \infty$ and that $\bar{x}$ and $\bar{y}$ are linear vector functions of $z$ where the parameters are estimated using ordinary least squares. Assume that $\|\bar{x}\|_{X}, \|\bar{y}\|_{Y} < c < \infty$ almost surely. Let $\eta_{\delta,N}$ be as defined in Definition 1. Then

$$\eta_{\delta,N} = O \left( \sqrt{\frac{d_{z}}{N}} \log((d_{x} + d_{y})/\delta) \right)$$

*Proof.* (sketch) This is based on results that bound parameter estimation error in linear regression with univariate response (e.g. [11]). Note that if $\bar{x}_{t_{i}} = U_{i}^{\top}z_{t}$ for
some $U_i \in Z$, then a bound on the error norm $\|\hat{U}_i - U_i\|$ implies a uniform bound of the same rate on $\hat{x}_i - \bar{x}$. The probability of exceeding the bound is scaled by $1/(d_x + d_y)$ to correct for multiple regressions.

Variants of Proposition 3 can also be developed using bounds on non-linear regression models (e.g., generalized linear models).

The next proposition addresses a scenario where $X$ and $Y$ are infinite dimensional.

**Proposition 4.** Assume that $x$ and $y$ are kernel evaluation functionals, $\bar{x}$ and $\bar{y}$ are linear vector functions of $z$ where the linear operator is estimated using conditional mean embedding [21] with regularization parameter $\lambda_0 > 0$ and that $\|\bar{x}\|_X, \|\bar{y}\|_Y < c < \infty$ almost surely. Let $\eta_{\delta,N}$ be as defined in Definition 1. It follows that

$$\eta_{\delta,N} = O\left(\sqrt{\lambda_0} + \sqrt{\frac{\log(N/\delta)}{\lambda_0 N}}\right).$$

**Proof:** (sketch) This bound is based on [21], which gives a bound on the error in estimating the conditional mean embedding. The error probability is adjusted by $\delta/4N$ to accommodate the requirement that the bound holds for all training data.

In the following, we apply theorem 2 to the setting of learning dynamical systems, where $Q_t \in X$, $P_t \in Y$ and $h_t \in Z$ ($Q_t$, $P_t$ and $h_t$ are as defined in Section 2). One issue to note is that theorem 2 assumes that the test input lies within $R(\Sigma_{xx})$. In dynamical systems context, however, the test input is an estimated predictive state $\hat{Q}_t$. Since S1 regression can fail to identify the subspace of true states given finite data, $\hat{Q}_t$ can have a non-zero component $\epsilon_t$ in $R(\Sigma_{xx})$, the orthogonal complement of $R(\Sigma_{xx})$. The following lemma states that, in a stable system, this component gets smaller as S1 regression performs better.

**Lemma 5.** For a test sequence $o_1:T$, let $\hat{Q}_t$ denote the estimated state given $o_{1:t-1}$. Let $\tilde{Q}_t$ denote the projection of $\hat{Q}_t$ onto $R(\Sigma_{xx})$. Assume that $f_{\text{filter}}$ is $L$-Lipchitz continuous on $P_t$ and that $f_{\text{filter}}(P_t, o_t) \in R(\Sigma_{xx})$ for any $P_t \in R(\Sigma_{yy})$. Given the assumptions in theorem 2 and assuming that $\|\hat{Q}_t\|_X \leq R$ for all $1 \leq t \leq T$, the following holds for all $1 \leq t \leq T$ with probability at least $1 - \delta/2$.

$$\|\epsilon_t\|_X = \|\hat{Q}_t - \tilde{Q}_t\|_X = O\left(\frac{\eta_{\delta,N}}{\sqrt{\lambda}}\right).$$
Since $\hat{W}_\lambda$ is bounded. The prediction error due to adding $\epsilon_t$ to the input diminishes at the same rate of $\|\epsilon_t\|_X$.

5 Case Study: Learning A Knowledge Tracing Model

In this section we demonstrate that we can learn a hidden Markov model using the two stage regression framework. We also demonstrate that we can change the regression methods to gain advantage. Specifically, we consider a limited data scenario, where we have a conflict between using many history features (picking a long history window to reduce noise in our predictions, and rich features of that window to achieve a linear relationship between history and future) or using few history features (reducing the number of parameters we have to learn from limited data). We show that we can use non-linear S1 regression models to reduce the number of parameters we need to learn, resulting in better empirical prediction accuracy compared to linear models while still maintaining consistency.

In this experiment we attempt to model and predict the performance of students learning from an interactive computer-based tutor. We use the Bayesian knowledge tracing (BKT) model [8], which is essentially a 2-state HMM: the state $s_t$ represents whether a student has learned a knowledge component (KC), and the observation $o_t$ represents the success/failure of solving the $t^{th}$ question in a sequence of question that cover the said KC. With high probability, the student remains in the same state (learned or unlearned) and with smaller probability, the student may transition from unlearned to learned (learning) or learned to unlearned (forgetting). In the learned state, the student is more likely to answer a question correctly than in the unlearned state. It is also possible for the student to answer a question correctly while in the unlearned state (guessing) or incorrectly while in the learned state (slipping). The possible transitions and observations are summarized in figure 3.

5.1 Data Description

The data set we used to evaluate the model is a publicly available data set from DataShop [15] called “Geometry Area (1996-97).” This data was generated by students learning introductory geometry, and contains attempts by 59 students in 12 knowledge components. As is typical for BKT, we consider a student’s attempt at a question to be correct iff the student entered the correct answer on the first try, without requesting any hints from the help system. The sequence of first attempts
Figure 3: Transitions and observation emissions of the BKT model. (Each node represents a possible value of the state/observation). Solid arrows represent transitions while dashed arrows represent emissions. Horizontal arrows represent “ordinary” transitions and emissions, where skill level is maintained and correctly represented by the answer. Diagonal arrows represent emissions where the student guessed or slipped, or transitions where the student learned or forgot the skill.
for a student/KC pair constitutes a training sequence. We discard sequences of length less than 5, resulting in a total of 325 sequences. We pad each observation sequence at the beginning with dummy observations, to handle the case where the history window extends before the beginning of the sequence. (This procedure allows us to use more data in our regressions, which is important because of our limited sample size.) Therefore a history observation which is used as training input for $S_1$ regression can be in one of three states: “correct”, “incorrect” or “before beginning of time.” We restrict the regression output however to be binary (“correct” or “incorrect”).

5.2 Model Description

Under the (reasonable) assumption that the two states have distinct observation probabilities, this model is 1-observable. It is reasonable then to choose the predictive state to be the expected next observation, which results in the following statistics:

$$
\psi_t = o_t \\
\xi_t = o_t \otimes_k o_{t+1},
$$

where $o_t$ is represented by a 2 dimensional indicator vector and $\otimes_k$ denotes the Kronecker product. Given these statistics, $P_t = \mathbb{E}[\xi_t | o_1:t-1]$ is a joint probability table of $o_{t:t+1}$ from which conditioning on $o_t$ (filtering) and marginalizing over $o_t$ (prediction) are simple operations. It thus remains to choose the history features $h_t$ and the $S_1$ regression model. In the appendix, we show that if use $h_t = o_{t-1}$ and linear regression as $S_1$ regression model, the resulting algorithm is equivalent to spectral HMM method of [10] and thus we use it as a baseline. In fact, if we had access to sufficient data, we could learn the HMM using this base line model. Not counting dummy observations, the model has to learn 7 parameters (7 free covariance entries). Under limited data, however, we can achieve faster learning by incorporating prior knowledge. Here, we will take advantage of the intuition that switching states (learning or forgetting) is a relatively unlikely event. Hence, aggregating observations over multiple previous time steps is a better predictor of the state, since aggregation will mitigate the effects of guessing and slipping. So we would like to use $h_t = o_{t-b:t-1}$ for some $b > 1$. We then have a choice: if we represent $h_t$ by an indicator vector of dimension $2^b$, then the optimal predictor of $o_t$ from $h_t$ will be linear, but the number of parameters we must learn will increase exponentially with $b$. On the other hand, if we represent $h_t$ by a binary vector of
| Model  | S1 Regression | History Features |
|--------|---------------|------------------|
| model 1 | Linear        | $o_{t-1}$        |
| model 2 | Linear        | $o_{t-4:t-1}$ (Indicator) |
| model 3 | Logistic      | $o_{t-4:t-1}$ (Separate) |

Table 1: Evaluated models: “indicator” means we have one feature for each distinct sequence of length $b$, while “separate” means that we have separate discrete features for each observation in the history window.

length $b$, then we will only need to learn $b + 1$ parameters, but the optimal predictor of $o_t$ from $h_t$ will no longer be linear leading to poor performance of linear regression. It is not obvious a priori which choice will result in better learning performance.\(^5\)

Our formulation makes the choice much easier: we can use a history window of any length, pick the more-concise length-$b$ representation, and train a nonlinear predictor such as a logistic regression. By doing so we combine the advantages of both of the previous paragraph’s approaches: we only need to learn $O(b)$ parameters, but our class of predictors still includes a near-optimal choice. (Logistic regression becomes exactly optimal as the probabilities of learning and forgetting approach zero. Since these probabilities are typically small in practice, logistic regression will be close to optimal in practice.) As we will see below, the result is better learning from limited data.

### 5.3 Evaluation Procedure and Results

We evaluated three variants of HMM learning via two-stage regression. They are summarized in Table 1. We evaluated the models using 1000 random splits of the 325 sequences into 200 training and 125 testing. For each split, we trained each model on the training sequences. Then for each test sequence, we filter through the first 3 observations then predict the rest of the sequence, reporting the root mean square error for each split. The results are depicted in figure 4. The results show that, in terms of accuracy, model 3 outperforms model 2, which in turn outperforms model 1. In other words, feature expansion does increase predictive accuracy. However, even more gain is achieved using non-linear S1 models that require fewer parameters.

\(^5\)The numbers above ignore the effect of padding observation sequences, but the conclusions are similar in either case.
Figure 4: Experimental results: each graph depicts the performance of two models (measured by RMSE) on 1000 train/test splits. The black line represents the $x = y$ lines. More points below the line indicates that model y is better than model x.
6 Conclusion

In this work we developed a general framework for dynamical system learning using supervised learning methods. The proposed framework is based on two-stage regression: in the first stage we use history features to train regression models that denoise future observation windows into state estimates. In the second stage we use these state estimates to train a linear model that represents system dynamics.

This framework encompasses and provides a unified view of some successful dynamical system learning algorithms. We demonstrated the proposed framework in learning a Hidden Markov Model, where we have shown that we can use nonlinear regression to incorporate more history features in identifying the latent state without an exponential increase in the number of parameters.

As future work, we would like to apply this framework to more scenarios where we can leverage additional techniques such as manifold embedding, sparse learning and transfer learning in stage 1 regression. We would also like to extend the framework to controlled processes.

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A Spectral and HSE Dynamical System Learning as Regression

In this section we provide examples of mapping some of the successful dynamical system learning algorithms to our framework.

A.1 HMM

In this section we show that we can use instrumental regression framework to reproduce the spectral learning algorithm for learning HMM [10]. We consider 1-observable models but the argument applies to $k$-observable models. In this case we use $\psi_t = e_{o_t}$ and $\xi_t = e_{o_t,t+1} = e_{o_t} \otimes_k e_{o_{t+1}}$, where $\otimes_k$ denotes the kronecker product. Let $P_{i,j} \equiv \mathbb{E}[e_{o_i} \otimes e_{o_j}]$ be the joint probability table of observations $i$ and $j$ and let $\hat{P}_{i,j}$ be its estimate from the data. We start with the (very restrictive) case where $P_{1,2}$ is invertible. Given samples of $h_2 = e_{o_1}$, $\psi_2 = e_{o_2}$ and $\xi_2 = e_{o_{2,3}}$, in S1 regression we apply linear regression to learn two matrices $\hat{W}_{2,1}$ and $\hat{W}_{2,3,1}$ such that:

$$
\mathbb{E}[\psi_2|h_2] = \Sigma_{o_{2,1}} \Sigma_{o_1}^{-1} h_2 = \hat{P}_{2,1}^{-1} \hat{P}_{1,1} h_2 \equiv \hat{W}_{2,1} h_2 \quad (A.1)
$$

$$
\mathbb{E}[\xi_2|h_2] = \Sigma_{o_{2,3}o_1} \Sigma_{o_1}^{-1} h_2 = \hat{P}_{2,3,1}^{-1} \hat{P}_{1,1} h_2 \equiv \hat{W}_{2,3,1} h_2, \quad (A.2)
$$

where $P_{2:3,1} \equiv \mathbb{E}[e_{o_{2,3}} \otimes e_{o_1}]$

In S2 regression, we learn the matrix $\hat{W}$ that gives the least squares solution to the system of equations

$$
\mathbb{E}[\xi_2|h_2] \equiv \hat{W}_{2,3,1} e_{o_1} = \hat{W}(\hat{W}_{2,1} e_{o_1}) \equiv \hat{W} \mathbb{E}[\psi_2|h_2], \quad \text{for given samples of } h_2
$$

which gives

$$
\hat{W} = \hat{W}_{2:3,1} \mathbb{E}[e_{o_1} e_{o_1}^\top] \hat{W}_{2,1}^\top \left( \hat{W}_{2,1} \mathbb{E}[e_{o_1} e_{o_1}^\top] \hat{W}_{2,1}^\top \right)^{-1} = \left( \hat{P}_{2:3,1} \hat{P}_{1,1}^{-1} \hat{P}_{2,1}^\top \right) \left( \hat{P}_{2,1} \hat{P}_{1,1}^{-1} \hat{P}_{2,1}^\top \right)^{-1} = \hat{P}_{2:3,1} \hat{P}_{2,1}^{-1} \quad (A.3)
$$

Having learned the matrix $\hat{W}$, we can estimate

$$
\hat{P}_t \equiv \hat{W} Q_t
$$
starting from a state \( Q_t \). Since \( P_t \) specifies a joint distribution over \( e_{o_{t+1}} \) and \( e_{o_t} \), we can easily condition on (or marginalize \( o_t \)) to obtain \( Q_{t+1} \). We will show that this is equivalent to learning and applying observable operators as in [10]:

For a given value \( x \) of \( o_2 \), define

\[
B_x = u_x^\top \hat{W} = u_x^\top \hat{P}_{2:3,1} \left( \hat{P}_{2,1}^\top \right)^{-1},
\]

where \( u_x \) is an \(|\mathcal{O}| \times |\mathcal{O}|^2 \) matrix which selects a block of rows in \( \hat{P}_{2:3,1} \) corresponding to \( o_2 = x \). Specifically, \( u_x = \delta_x \otimes_k I_{|\mathcal{O}|} \).

\[
Q_{t+1} = \hat{E}[\delta \mid o_{t+1}^\top o_{t+1}] \propto u_{o_t} \hat{E}[\delta \mid o_{t+1}^\top o_{t-1}]
\]

\[
= u_{o_t} \hat{E}[\xi_t \mid o_{t-1}] = u_{o_t} \hat{W} \hat{E}[\psi_t \mid o_{t-1}] = B_{o_t} Q_t
\]

with a normalization constant given by

\[
\frac{1}{1^\top B_{o_t} Q_t}
\]

Now we move to a more realistic setting, where we have \( \text{rank}(P_{2,1}) = m < |\mathcal{O}| \). Therefore we project the predictive state using a matrix \( U \) that preserves the dynamics, by requiring that \( U^\top O \) (i.e. \( U \) is an independent set of columns spanning the range of the HMM observation matrix \( O \)).

It can be shown [10] that \( R(O) = R(P_{2,1}) = R(P_{2,1} P_{1,1}^{-1}) \). Therefore, we can use the leading \( m \) left singular vectors of \( \hat{W}_{2,1} \), which corresponds to replacing the linear regression in S1A with a reduced rank regression. However, for the sake of our discussion we will use the singular vectors of \( P_{2,1} \). In more detail, let \([U, S, V]\) be the rank-\( m \) SVD decomposition of \( P_{2,1} \). We use \( \psi_t = U^\top e_{o_t} \) and \( \xi_t = e_{o_t} \otimes_k U^\top e_{o_{t+1}} \). S1 weights are then given by \( \hat{W}_{2,1}^\text{rr} = U^\top \hat{W}_{2,1} \) and \( \hat{W}_{2:3,1}^\text{rr} = (I_{|\mathcal{O}|} \otimes_k U^\top) \hat{W}_{2:3,1} \) and S2 weights are given by

\[
\hat{W}_{2:3,1}^\text{rr} = (I_{|\mathcal{O}|} \otimes_k U^\top) \hat{W}_{2:3,1} \hat{E}[e_{o_t} e_{o_{t+1}}^\top] \hat{W}_{2,1}^\top U \left( U^\top \hat{W}_{2,1} \hat{E}[e_{o_t} e_{o_{t+1}}^\top] \hat{W}_{2,1}^\top U \right)^{-1}
\]

\[
= (I_{|\mathcal{O}|} \otimes_k U^\top) \hat{P}_{2:3,1} \hat{P}_{1,1}^{-1} V S \left( S V^\top \hat{P}_{1,1}^{-1} V S \right)^{-1}
\]

\[
= (I_{|\mathcal{O}|} \otimes_k U^\top) \hat{P}_{2:3,1} \hat{P}_{1,1}^{-1} V \left( V^\top \hat{P}_{1,1}^{-1} V \right)^{-1} S^{-1}
\]

\[\text{(A.6)}\]

\footnote{Following the notation used in [10], \( u_x^\top \hat{P}_{2:3,1} = \hat{P}_{3,x,1} \)}
In the limit of infinite data, $V$ spans $\text{range}(O) = \text{rowspace}(P_{2:3,1})$ and hence $P_{2:3,1} = P_{2:3,1}VV^T$. Substituting in (A.6) gives

$$W^{rr} = (I_{|\mathcal{O}|} \otimes_k U^T) P_{2:3,1} V S^{-1} = (I_{|\mathcal{O}|} \otimes_k U^T) P_{2:3,1} (U^T P_{2,1})^+$$

Similar to the full-rank case we define, for each observation $x$ an $m \times |\mathcal{O}|^2$ selector matrix $u_x = \delta_x \otimes_k I_m$ and an observation operator

$$B_x = u_x^T \hat{W}^{rr} \rightarrow U^T P_{3,x,1} (U^T P_{2,1})^+ \quad (A.7)$$

This is exactly the observation operator obtained in [10]. However, instead of using A.6, they use A.7 with $P_{3,x,1}$ and $P_{2,1}$ replaced by their empirical estimates.

Note that for a state $b_t = \mathbb{E}[\psi_t | o_{1:t-1}]$, $B_x b_t = P(o_t | o_{1:t-1}) \mathbb{E}[\psi_{t+1} | o_{1:t}] = P(o_t | o_{1:t-1}) b_{t+1}$. To get $b_{t+1}$, the normalization constant becomes $\frac{1}{b_{t}^\top B_x b_t}$, where $b_{t+1}^\top b = 1$ for any valid predictive state $b$. To estimate $b_{\infty}$ we solve the aforementioned condition for states estimated from all possible values of history features $h_t$. This gives,

$$b_{\infty}^\top \hat{W}^{rr}_2 I_{|\mathcal{O}|} = b_{\infty}^\top U^T \hat{P}_{2,1} \hat{P}_{1,1}^{-1} I_{|\mathcal{O}|} = 1_{|\mathcal{O}|}^\top,$$

where the columns of $I_{|\mathcal{O}|}$ represent all possible values of $h_t$. This in turn gives

$$b_{\infty}^\top = 1_{|\mathcal{O}|}^\top \hat{P}_{1,1} (U^T \hat{P}_{2,1})^+ = \hat{P}_{i,1}^T (U^T \hat{P}_{2,1})^+,$$

the same estimator proposed in [10].

### A.2 Stationary Kalman Filter

A Kalman filter is given by

$$s_t = O s_{t-1} + \nu_t$$
$$o_t = T s_t + \epsilon_t$$
$$\nu_t \sim \mathcal{N}(0, \Sigma_{\nu})$$
$$\epsilon_t \sim \mathcal{N}(0, \Sigma_{\epsilon})$$
We consider the case of a stationary filter where $\Sigma_t \equiv \mathbb{E}[s_t s_t^T]$ is independent of $t$. We choose our statistics

$$
\begin{align*}
  h_t &= o_{t-H:t-1} \\
  \psi_t &= o_{t:t+F-1} \\
  \xi_t &= o_{t:t+F}
\end{align*}
$$

It can be shown [2, 25] that

$$
\mathbb{E}[s_t | h_t] = \Sigma_{s,h} \Sigma_{h,h}^{-1} h_t
$$

and it follows that

$$
\begin{align*}
  \mathbb{E}[\psi_t | h_t] &= \Gamma \Sigma_{s,h} \Sigma_{h,h}^{-1} h_t = W_1 h_t \\
  \mathbb{E}[\xi_t | h_t] &= \Gamma_+ \Sigma_{s,h} \Sigma_{h,h}^{-1} h_t = W_2 h_t
\end{align*}
$$

where $\Gamma$ is the extended observation operator

$$
\Gamma \equiv \begin{pmatrix} O \\ OT \\ \vdots \\ OT^F \end{pmatrix}, \quad \Gamma_+ \equiv \begin{pmatrix} O \\ OT \\ \vdots \\ OT^{F+1} \end{pmatrix}
$$

It follows that $F$ and $H$ must be large enough to have $\text{rank}(W) = n$. Let $U \in \mathbb{R}^{mF \times n}$ be the matrix of left singular values of $W_1$ corresponding to non-zero singular values. Then $U^T \Gamma$ is invertible and we can write

$$
\begin{align*}
  \mathbb{E}[\psi_t | h_t] &= U U^T \Gamma \Sigma_{s,h} \Sigma_{h,h}^{-1} h_t = W_1 h_t \\
  \mathbb{E}[\xi_t | h_t] &= \Gamma_+ \Sigma_{s,h} \Sigma_{h,h}^{-1} h_t = W_2 h_t \\
  \mathbb{E}[\xi_t | h_t] &= \Gamma_+ (U^T \Gamma)^{-1} U^T (U U^T \Gamma \Sigma_{s,h} \Sigma_{h,h}^{-1} h_t) \\
  &= W \mathbb{E}[\psi_t | h_t]
\end{align*}
$$

which matches the instrumental regression framework. For the steady-state case (constant Kalman gain), one can estimate $\Sigma_\xi$ given the data and the parameter $W$ by solving Riccati equation as described in [25]. $\mathbb{E}[\xi_t | o_{1:t-1}]$ and $\Sigma_\xi$ then specify a joint Gaussian distribution where marginalization and conditioning can be easily performed.
A.3 HSE-PSR

We define a class of non-parametric two-stage instrumental regression models. By using conditional mean embedding [21] as S1 regression model, we recover a single-action variant of HSE-PSR [5]. Let $\mathcal{X}, \mathcal{Y}, \mathcal{Z}$ denote three reproducing kernel Hilbert spaces with reproducing kernels $k_\mathcal{X}, k_\mathcal{Y}$ and $k_\mathcal{Z}$ respectively. Assume $\psi_t \in \mathcal{X}$ and that $\xi_t \in \mathcal{Y}$ is defined as the tuple $(o_t \otimes o_t, \psi_{t+1} \otimes o_t)$. Let $\Psi \in \mathcal{X} \otimes \mathbb{R}^N$, $\Xi \in \mathcal{Y} \otimes \mathbb{R}^N$ and $H \in \mathcal{Z} \otimes \mathbb{R}^N$ be operators that represent training data. Specifically, $\psi_s, \xi_s, h_s$ are the $s^{th}$ ”columns” in $\Psi$ and $\Xi$ and $H$ respectively. It is possible to implement S1 using a non-parametric regression method that takes the form of a linear smoother. In such case the training data for S2 regression take the form

$$\hat{E}[\psi_t \mid h_t] = \sum_{s=1}^{N} \beta_{s|h_t} \psi_s$$

$$\hat{E}[\xi_t \mid h_t] = \sum_{s=1}^{N} \gamma_{s|h_t} \xi_s,$$

where $\beta_s$ and $\gamma_s$ depend on $h_t$. This produces the following training operators for S2 regression:

$$\tilde{\Psi} = \Psi B$$

$$\tilde{\Xi} = \Xi \Gamma,$$

where $B_{st} = \beta_{s|h_t}$ and $\Gamma_{st} = \gamma_{s|h_t}$. With this data, S2 regression uses a Gram matrix formulation to estimate the operator

$$W = \Xi \Gamma (B^\top G_{\mathcal{X},\mathcal{X}} B + \lambda I_N)^{-1} B^\top \Psi^*$$

(A.8)

Note that we can use an arbitrary method to estimate $B$. Using conditional mean maps, the weight matrix $B$ is computed using kernel ridge regression

$$B = (G_{\mathcal{Z},\mathcal{Z}} + \lambda I_N)^{-1} G_{\mathcal{Z},\mathcal{Z}}$$

(A.9)

HSE-PSR learning is similar to this setting, with $\psi_t$ being a conditional expectation operator of test observations given test actions. For this reason, kernel ridge regression is replaced by application of kernel Bayes rule [9].
For each \( t \), S1 regression will produce a denoised prediction \( \hat{E}[\xi_t \mid h_t] \) as a linear combination of training feature maps

\[
\hat{E}[\xi_t \mid h_t] = \Xi \alpha_t = \sum_{s=1}^{N} \alpha_{t,s} \xi_s
\]

This corresponds to the covariance operators

\[
\hat{\Sigma}_{\psi_{t+1} \alpha_t|h_t} = \sum_{s=1}^{N} \alpha_{t,s} \psi_{s+1} \otimes o_s = \Psi' \text{diag}(\alpha_t) \mathbf{O}^*
\]

\[
\hat{\Sigma}_{o_t \alpha_t|h_t} = \sum_{s=1}^{N} \alpha_{t,s} o_s \otimes o_s = \mathbf{O} \text{diag}(\alpha_t) \mathbf{O}^*
\]

Where, \( \Psi' \) is the shifted future training operator satisfying \( \Psi' e_t = \psi_{t+1} \). Given these two covariance operators, we can use kernel Bayes rule [9] to condition on \( o_t \) which gives

\[
Q_{t+1} = \hat{E}[\psi_{t+1} \mid h_t] = \hat{\Sigma}_{\psi_{t+1} \alpha_t|h_t} (\hat{\Sigma}_{o_t \alpha_t|h_t} + \lambda \mathbf{I})^{-1} o_t. \tag{A.10}
\]

Replacing \( o_t \) in (A.10) with its conditional expectation \( \sum_{s=1}^{N} \alpha_s o_s \) corresponds to marginalizing over \( o_t \) (i.e. prediction). A stable Gram matrix formulation for (A.10) is given by [9]

\[
Q_{t+1} = \Psi' \text{diag}(\alpha_t) G_{\sigma,\mathcal{O}} (\text{diag}(\alpha_t) G_{\sigma,\mathcal{O}}^2 + \lambda N \mathbf{I})^{-1} \text{diag}(\alpha_t) \mathbf{O}^* o_{t+1}
\]

\[
= \Psi' \tilde{\alpha}_{t+1}, \tag{A.11}
\]

which is the state update equation in HSE-PSR. Given \( \tilde{\alpha}_{t+1} \) we perform S2 regression to estimate

\[
\hat{P}_{t+1} = \hat{E}[\xi_{t+1} \mid o_{1:t+1}] = \Xi \alpha_{t+1} = W \Psi' \tilde{\alpha}_{t+1},
\]

where \( W \) is defined in (A.8).
B Proofs

B.1 Proof of Main Theorem

In this section we provide a proof for theorem 2. We provide finite sample analysis of the effects of S1 regression, covariance estimation and regularization. The asymptotic statement becomes a natural consequence.

We will make use of matrix Bernstein’s inequality stated below:

**Lemma B.1** (Matrix Bernstein’s Inequality [12]). Let $A$ be a random square symmetric matrix, and $r > 0$, $v > 0$ and $k > 0$ be such that, almost surely,

\[
\mathbb{E}[A] = 0, \quad \lambda_{\text{max}}[A] \leq r, \\
\lambda_{\text{max}}[\mathbb{E}[A^2]] \leq v, \quad \text{tr}(\mathbb{E}[A^2]) \leq k.
\]

If $A_1, A_2, \ldots, A_N$ are independent copies of $A$, then for any $t > 0$,

\[
\Pr \left[ \lambda_{\text{max}} \left( \frac{1}{N} \sum_{t=1}^{N} A_t \right) > \sqrt{\frac{2vt}{N} + \frac{rt}{3N}} \right] \leq \frac{kt}{v}(e^t - t - 1)^{-1}. \tag{B.1}
\]

If $t \geq 2.6$, then $t(e^t - t - 1)^{-1} \leq e^{-t/2}$.

Recall that, assuming $x_{\text{test}} \in \mathcal{R}(\Sigma_{\tilde{x}\tilde{x}})$, we have three sources of error: first, the error in S1 regression causes the input to S2 regression procedure $(\hat{x}_t, \hat{y}_t)$ to be a perturbed version of the true $(\bar{x}_t, \bar{y}_t)$; second, the covariance operators are estimated from a finite sample of size $N$; and third, there is the effect of regularization. In the proof, we characterize the effect of each source of error. To do so, we define the following intermediate quantities:

\[
W_\lambda = \Sigma_{\tilde{y}\tilde{x}} \left( \Sigma_{\tilde{x}\tilde{x}} + \lambda I \right)^{-1}, \tag{B.2}
\]

\[
\tilde{W}_\lambda = \tilde{\Sigma}_{\tilde{y}\tilde{x}} \left( \tilde{\Sigma}_{\tilde{x}\tilde{x}} + \lambda I \right)^{-1}, \tag{B.3}
\]

where

\[
\tilde{\Sigma}_{\tilde{y}\tilde{x}} \equiv \frac{1}{N} \sum_{t=1}^{N} \tilde{y}_t \otimes \tilde{x}_t
\]
and $\hat{\Sigma}_{xx}$ is defined similarly. Basically, $W_\lambda$ captures only the effect of regularization and $\bar{W}_\lambda$ captures in addition the effect of finite sample estimate of the covariance. $W_\lambda$ is the result of S2 regression if $\bar{x}$ and $\bar{y}$ were perfectly recovered by S1 regression. It is important to note that $\hat{\Sigma}_{x\bar{y}}$ and $\hat{\Sigma}_{xx}$ are not observable quantities since they depend on the true expectations $\bar{x}$ and $\bar{y}$. We will use $\lambda_{x1}$ and $\lambda_{y1}$ to denote the $i^{th}$ eigenvalue of $\Sigma_{xx}$ and $\Sigma_{yy}$ respectively in descending order and we will use $\|\cdot\|$ to denote the operator norm.

Before we prove the main theorem, we define the quantities $\zeta_{x\bar{x},\delta,N}$ and $\zeta_{x\bar{y},\delta,N}$ which we use to bound the effect of covariance estimation from finite data, as stated in the following lemma:

**Lemma B.2** (Covariance error bound). Let $N$ be a positive integer and $\delta \in (0, 1)$ and assume that $\|\bar{x}\|, \|\bar{y}\| < c < \infty$ almost surely. Let $\zeta_{x\bar{y},\delta,N}$ be defined as:

$$\zeta_{x\bar{y},\delta,N} = \sqrt{\frac{2v}{N} + \frac{rt}{3N}},$$

(B.4)

where

$$t = \max(2.6, 2\log(4k/\delta v))$$
$$r = c^2 + \|\hat{\Sigma}_{y\bar{x}}\|$$
$$v = c^2 \max(\lambda_{y1}, \lambda_{x1}) + \|\hat{\Sigma}_{x\bar{y}}\|^2$$
$$k = c^2 (\text{tr}(\hat{\Sigma}_{xx}) + \text{tr}(\hat{\Sigma}_{y\bar{y}}))$$

In addition, let $\zeta_{x\bar{x},\delta,N}$ be defined as:

$$\zeta_{x\bar{x},\delta,N} = \sqrt{\frac{2v't'}{N} + \frac{r't'}{3N}},$$

(B.5)

where

$$t' = \max(2.6, 2\log(4k'/\delta v'))$$
$$r' = c^2 + \lambda_{x1}$$
$$v' = c^2 \lambda_{x1} + \lambda_{x1}^2$$
$$k' = c^2 \text{tr}(\hat{\Sigma}_{xx})$$

and define $\zeta_{y\bar{y},\delta,N}$ similarly for $\Sigma_{y\bar{y}}$. 

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It follows that, with probability at least $1 - \delta/2$,
\[
\|\hat{\Sigma}_{\bar{y}\bar{x}} - \Sigma_{\bar{y}\bar{x}}\| < \zeta_{\delta, N}
\]
\[
\|\hat{\Sigma}_{\bar{x}\bar{x}} - \Sigma_{\bar{x}\bar{x}}\| < \zeta_{\delta, N}
\]
\[
\|\hat{\Sigma}_{\bar{y}\bar{y}} - \Sigma_{\bar{y}\bar{y}}\| < \zeta_{\delta, N}
\]

**Proof.** We show that each statement holds with probability at least $1 - \delta/6$. The claim then follows directly from the union bound. We start with $\zeta_{\delta, N}$. By setting $A_t = \bar{x}_t \otimes \bar{x}_t - \Sigma_{\bar{x}\bar{x}}$ then we would like to obtain a high probability bound on $\|\frac{1}{N} \sum_{t=1}^N A_t\|$. Lemma B.1 shows that, in order to satisfy the bound with probability at least $1 - \delta/6$, it suffices to set $t$ to $\max(2.6, 2k \log(6/\delta v))$. So, it remains to find suitable values for $r, v$ and $k$:

\[
\lambda_{\max}[A] \leq \|\bar{x}\|^2 + \|\Sigma_{\bar{x}\bar{x}}\| \leq c^2 + \lambda_{x1} = r'
\]
\[
\lambda_{\max}[\mathbb{E}[A^2]] = \lambda_{\max}[\mathbb{E}[\|\bar{x}\|^2(\bar{x} \otimes \bar{x}) - (\bar{x} \otimes \bar{x})\Sigma_{\bar{x}\bar{x}} - \Sigma_{\bar{x}\bar{x}}(\bar{x} \otimes \bar{x}) + \Sigma_{\bar{x}\bar{x}}^2]] = c^2\lambda_{x1} + \lambda_{x1}^2 = v'
\]
\[
\text{tr}[\mathbb{E}[A^2]] = \text{tr}[\mathbb{E}[\|\bar{x}\|^2(\bar{x} \otimes \bar{x}) - \Sigma_{\bar{x}\bar{x}}^2]] \leq \text{tr}[\mathbb{E}[\|\bar{x}\|^2(\bar{x} \otimes \bar{x})]] \leq c^2\text{tr}(\Sigma_{\bar{x}\bar{x}}) = k'
\]

The case of $\zeta_{\delta, N}$ can be proven similarly. Now moving to $\zeta_{\delta, N}$, we have $B_t = \bar{y}_t \otimes \bar{x}_t - \Sigma_{\bar{y}\bar{x}}$. Since $B_t$ is not square, we use the Hermitian dilation $\mathcal{H}(B)$ defined as follows[24]:

\[
A = \mathcal{H}(B) = \begin{bmatrix} 0 & B \\ B^* & 0 \end{bmatrix}
\]

Note that

\[
\lambda_{\max}[A] = \|B\|, \quad A^2 = \begin{bmatrix} BB^* & 0 \\ 0 & B^*B \end{bmatrix}
\]

therefore suffices to bound $\|\frac{1}{N} \sum_{t=1}^N A_t\|$ using an argument similar to that used in $\zeta_{\delta, N}$ case. \hfill \Box

To prove theorem 2, we write
\[
\|\hat{W}_\lambda x_{\text{test}} - W x_{\text{test}}\|_Y \leq \|(\hat{W}_\lambda - W_\lambda)\Hat{x}_{\text{test}}\|_Y
\]
\[
+ \|(W_\lambda - W_\lambda)\Hat{x}_{\text{test}}\|_Y
\]
\[
+ \|(W_\lambda - W)\Hat{x}_{\text{test}}\|_Y \tag{B.6}
\]
We will now present bounds on each term. We consider the case where \( \bar{x}_{\text{test}} \in \mathcal{R}(\Sigma_{xx}) \). Extension to \( \mathcal{R}(\Sigma_{g\bar{y}}) \) is a result of the assumed boundedness of \( W \), which implies the boundedness of \( \hat{W}_\lambda - W \).

**Lemma B.3 (Error due to S1 Regression).** Assume that \( \|\bar{x}\|, \|\bar{y}\| < c < \infty \) almost surely, and let \( \eta_{\delta,N} \) be as defined in Definition 1. The following holds with probability at least \( 1 - \delta \)

\[
\|\hat{W}_\lambda - \check{W}_\lambda\| \leq \sqrt{\frac{\lambda y_t + \zeta_{\delta,N}^y (2c\eta_{\delta,N} + \eta_{\delta,N}^2)}{\lambda^2}} + \frac{(2c\eta_{\delta,N} + \eta_{\delta,N}^2)}{\lambda} \\
= O \left( \eta_{\delta,N} \left( \frac{1}{\lambda} + \sqrt{\frac{1 + \log(1/\delta)}{\lambda}} \right) \right). 
\]

The asymptotic statement assumes \( \eta_{\delta,N} \to 0 \) as \( N \to \infty \).

**Proof.** Write \( \hat{\Sigma}_{x\bar{x}} = \hat{\Sigma}_{x\bar{x}} + \Delta_x \) and \( \hat{\Sigma}_{g\bar{y}} = \hat{\Sigma}_{g\bar{y}} + \Delta_{yx} \). We know that, with probability at least \( 1 - \delta/2 \), the following is satisfied for all unit vectors \( \phi_x \in \mathcal{X} \) and \( \phi_y \in \mathcal{Y} \)

\[
\langle \phi_y, \Delta_{yx} \phi_x \rangle_Y = \frac{1}{N} \sum_{t=1}^{N} \langle \phi_y, \hat{y}_t \rangle_Y \langle \phi_x, \hat{x}_t \rangle_X \\
- \langle \phi_y, \hat{y}_t \rangle_Y \langle \phi_x, \bar{x}_t \rangle_X \\
+ \langle \phi_y, \hat{y}_t \rangle_Y \langle \phi_x, \bar{x}_t \rangle_X - \langle \phi_y, \bar{y}_t \rangle_Y \langle \phi_x, \bar{x}_t \rangle_X \\
= \frac{1}{N} \sum_{t} \langle \phi_y, \bar{y}_t + (\hat{y}_t - \bar{y}_t) \rangle_Y \langle \phi_x, \hat{x}_t - \bar{x}_t \rangle_X \\
+ \langle \phi_y, \hat{y}_t - \bar{y}_t \rangle_Y \langle \phi_x, \bar{x}_t \rangle_X \\
\leq 2c\eta_{\delta,N} + \eta_{\delta,N}^2 
\]

Therefore,

\[
\|\Delta_{yx}\| = \sup_{\|\phi_x\|, \|\phi_y\| \leq 1} \langle \phi_y, \Delta_{yx} \phi_x \rangle_Y \leq 2c\eta_{\delta,N} + \eta_{\delta,N}^2, 
\]

and similarly

\[
\|\Delta_x\| \leq 2c\eta_{\delta,N} + \eta_{\delta,N}^2, 
\]
with probability $1 - \delta/2$. We can write

$$
\hat{W}_\lambda - \hat{W}_\lambda = \hat{\Sigma}_{g\hat{\Sigma}} \left( (\hat{\Sigma}_{xx} + \Delta_x + \lambda I)^{-1} - (\hat{\Sigma}_{xx} + \lambda I)^{-1} \right)
+ \Delta_{yx} (\hat{\Sigma}_{xx} + \Delta_x + \lambda I)^{-1}
$$

Using the fact that $B^{-1} - A^{-1} = B^{-1}(A - B)A^{-1}$ for invertible operators $A$ and $B$ we get

$$
\hat{W}_\lambda - \hat{W}_\lambda = -\hat{\Sigma}_{g\hat{\Sigma}} (\hat{\Sigma}_{xx} + \lambda I)^{-1} \Delta_x (\hat{\Sigma}_{xx} + \Delta_x + \lambda I)^{-1}
+ \Delta_{yx} (\hat{\Sigma}_{xx} + \Delta_x + \lambda I)^{-1}
$$

we then use the decomposition $\hat{\Sigma}_{g\hat{\Sigma}} = \hat{\Sigma}_{g\hat{\Sigma}} V \hat{\Sigma}_{g\hat{\Sigma}}$, where $V$ is a correlation operator satisfying $\|V\| \leq 1$. This gives

$$
\hat{W}_\lambda - \hat{W}_\lambda =
- \hat{\Sigma}_{g\hat{\Sigma}} V \hat{\Sigma}_{g\hat{\Sigma}} (\hat{\Sigma}_{xx} + \lambda I)^{-\frac{1}{2}} (\hat{\Sigma}_{xx} + \lambda I)^{-\frac{1}{2}} \Delta_x (\hat{\Sigma}_{xx} + \Delta_x + \lambda I)^{-1}
+ \Delta_{yx} (\hat{\Sigma}_{xx} + \Delta_x + \lambda I)^{-1}
$$

Noting that $\| \hat{\Sigma}_{g\hat{\Sigma}} (\hat{\Sigma}_{xx} + \lambda I)^{-\frac{1}{2}} \| \leq 1$, the rest of the proof follows from triangular inequality and the fact that $\|AB\| \leq \|A\|\|B\|$. \hfill $\square$

**Lemma B.4** (Error due to Covariance). *Assuming that* $\|\vec{x}\|_{\mathcal{X}}, \|\vec{y}\|_{\mathcal{Y}} < c < \infty$ *almost surely, the following holds with probability at least $1 - \frac{\delta}{2}$

$$
\|\hat{W}_\lambda - W_\lambda\| \leq \sqrt{\lambda y^2 \zeta_{\delta,N}^2 \lambda^{-\frac{3}{2}}} + \frac{\zeta_{\delta,N}}{\lambda}
$$

*where* $\zeta_{\delta,N}$ *and* $\zeta_{\delta,N}^2$ *are as defined in Lemma B.2.*

**Proof.** Write $\hat{\Sigma}_{g\hat{\Sigma}} = \hat{\Sigma}_{xx} + \Delta_x$ *and* $\hat{\Sigma}_{g\hat{\Sigma}} = \Sigma_{g\hat{\Sigma}} + \Delta_{yx}$. Then we get

$$
\hat{W}_\lambda - W_\lambda = \Sigma_{g\hat{\Sigma}} \left( (\hat{\Sigma}_{xx} + \Delta_x + \lambda I)^{-1} - (\hat{\Sigma}_{xx} + \lambda I)^{-1} \right) + \Delta_{yx} (\hat{\Sigma}_{xx} + \Delta_x + \lambda I)^{-1}
$$

Using the fact that $B^{-1} - A^{-1} = B^{-1}(A - B)A^{-1}$ for invertible operators $A$ and $B$ we get

$$
\hat{W}_\lambda - W_\lambda = -\Sigma_{g\hat{\Sigma}} (\hat{\Sigma}_{xx} + \lambda I)^{-1} \Delta_x (\hat{\Sigma}_{xx} + \Delta_x + \lambda I)^{-1} + \Delta_{yx} (\hat{\Sigma}_{xx} + \Delta_x + \lambda I)^{-1}
$$
we then use the decomposition $\Sigma_{\tilde{y}\tilde{x}} = \Sigma_{\tilde{y}\tilde{y}}^{1/2} V \Sigma_{\tilde{x}\tilde{x}}^{1/2}$, where $V$ is a correlation operator satisfying $\|V\| \leq 1$. This gives

$$W_\lambda - W_\tilde{\lambda} = \right.
- \Sigma_{\tilde{y}\tilde{y}}^{1/2} V \Sigma_{\tilde{x}\tilde{x}}^{1/2} (\Sigma_{\tilde{x}\tilde{x}} + \lambda I)^{-1/2} (\Sigma_{\tilde{x}\tilde{x}} + \lambda I)^{-1/2}
+ \Delta_x (\Sigma_{\tilde{x}\tilde{x}} + \Delta_x + \lambda I)^{-1}
+ \Delta_{yx} (\Sigma_{\tilde{x}\tilde{x}} + \Delta_x + \lambda I)^{-1}

Noting that $\|\Sigma_{\tilde{x}\tilde{x}}^{1/2} (\Sigma_{\tilde{x}\tilde{x}} + \lambda I)^{-1/2}\| \leq 1$, the rest of the proof follows from triangular inequality and the fact that $\|AB\| \leq \|A\|\|B\|

Lemma B.5 (Error due to Regularization on inputs within $\mathcal{R}(\Sigma_{\tilde{x}\tilde{x}})$). For any $x \in \mathcal{R}(\Sigma_{\tilde{x}\tilde{x}})$ s.t. $\|x\|_\chi \leq 1$ and $\|\Sigma_{\tilde{x}\tilde{x}}^{-1/2} x\|_\chi \leq C$. The following holds

$$\|(W_\lambda - W)x\|_\psi \leq \frac{1}{2}\sqrt{\lambda} \|W\|_{HS} C$$

Proof. Since $x \in \mathcal{R}(\Sigma_{\tilde{x}\tilde{x}}) \subseteq \mathcal{R}(\Sigma_{\tilde{x}\tilde{x}}^{1/2})$, we can write $x = \Sigma_{\tilde{x}\tilde{x}}^{1/2} v$ for some $v \in \chi$ s.t. $\|v\|_\chi \leq C$. Then

$$(W_\lambda - W)x = \Sigma_{\tilde{y}\tilde{x}} (\Sigma_{\tilde{x}\tilde{x}} + \lambda I)^{-1} - \Sigma_{\tilde{x}\tilde{x}}^{-1} \Sigma_{\tilde{x}\tilde{x}}^{1/2} v$$

Let $D = \Sigma_{\tilde{y}\tilde{x}} (\Sigma_{\tilde{x}\tilde{x}} + \lambda I)^{-1} - \Sigma_{\tilde{x}\tilde{x}}^{-1/2}$. We will bound the Hilbert-Schmidt norm of $D$. Let $\psi_{xi} \in \chi$, $\psi_{yi} \in \psi$ denote the eigenvector corresponding to $\lambda_{xi}$ and $\lambda_{yi}$ respectively. Define $s_{ij} = |\langle \psi_{yi}, \Sigma_{\tilde{y}\tilde{x}}^{1/2} \psi_{xi} \rangle_\psi|$. Then we have

$$|\langle \psi_{yj}, D \psi_{xi} \rangle_\psi| = \left| \frac{\lambda}{(\lambda_{xi} + \lambda) \sqrt{\lambda_{xi}}} s_{ij} \right| = \frac{s_{ij}}{\sqrt{\lambda_{xi}}} \frac{1}{\lambda_{xi} + \lambda} + 1$$

$$\leq \frac{s_{ij}}{\sqrt{\lambda_{xi}}} \frac{1}{2} \sqrt{\frac{\lambda}{\lambda_{xi}}} \leq \frac{1}{2} \sqrt{\lambda} |\langle \psi_{yj}, W \psi_{xi} \rangle_\psi|.$$
where the inequality follows from the arithmetic-geometric-harmonic mean inequality. This gives the following bound
\[
\|D\|^2_{HS} = \sum_{i,j} \langle \psi_{yj}, D\psi_{xi} \rangle^2_Y \leq \frac{1}{2} \sqrt{\lambda} \|W\|^2_{HS}
\]
and hence
\[
\|(W\lambda - W)x\|_Y \leq \|D\|\|v\|_X \leq \|D\|_{HS} \|v\|_X \leq \frac{1}{2} \sqrt{\lambda} \|W\|_{HS} C
\]
Note that the additional assumption that \(\|\Sigma_{xx}^{-\frac{1}{2}}x\|_X \leq C\) is not required to obtain an asymptotic \(O(\sqrt{\lambda})\) rate for a given \(x\). This assumption, however, allows us to uniformly bound the constant. Theorem 2 is simply the result of plugging the bounds in Lemmata B.3, B.4, and B.5 into (B.6) and using the union bound.

B.2 Proof of Lemma 5
for \(t = 1\): Let \(\mathcal{I}\) be an index set over training instances such that
\[
\hat{Q}_{1\text{test}} = \frac{1}{|\mathcal{I}|} \sum_{i \in \mathcal{I}} \hat{Q}_i
\]
Then
\[
\|\hat{Q}_{1\text{test}} - \hat{Q}_{1\text{test}}\|_X = \frac{1}{|\mathcal{I}|} \sum_{i \in \mathcal{I}} \|\hat{Q}_i - \hat{Q}_i\|_X \leq \frac{1}{|\mathcal{I}|} \sum_{i \in \mathcal{I}} \|\hat{Q}_i - Q_i\|_X \leq \eta_{\delta,N}
\]
for \(t > 1\): Let \(A\) denote a projection operator on \(\mathcal{R}^\perp(\Sigma_{yy})\)
\[
\|\hat{Q}_{t+1\text{test}} - \hat{Q}_{t+1\text{test}}\|_X \leq L\|\hat{P}_{t\text{test}} - \hat{P}_{t\text{test}}\|_Y \leq L\|\hat{W}_\lambda \hat{Q}_{t\text{test}}\|_Y
\]
\[
\leq L \left\| \frac{1}{N} \left( \sum_{i=1}^N A\hat{P}_i \otimes \hat{Q}_i \right) \left( \frac{1}{N} \sum_{i=1}^N \hat{Q}_i \otimes \hat{Q}_i + \lambda I \right)^{-1} \right\|_X \|\hat{Q}_{t\text{test}}\|_X
\]
\[
\leq L \left\| \frac{1}{N} \sum_{i=1}^N A\hat{P}_i \otimes A\hat{P}_i \right\|_X \frac{1}{\sqrt{\lambda}} \frac{1}{\sqrt{\lambda}} \|\hat{Q}_{t\text{test}}\|_X \leq \frac{L \eta_{\delta,N}}{\sqrt{\lambda}} \|\hat{Q}_{t\text{test}}\|_X,
\]
where the second to last inequality follows from the decomposition similar to \(\Sigma_{YX} = \Sigma_{YV} \frac{1}{2} \Sigma_{X} \), and the last inequality follows from the fact that \(\|A\hat{P}_i\|_Y \leq \|P_i - \hat{P}_i\|_Y\).