Variance Estimation For Online Regression via Spectrum Thresholding

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Abstract

We consider the online linear regression problem, where the predictor vector may vary with time. This problem can be modelled as a linear dynamical system, where the parameters that need to be learned are the variance of both the process noise and the observation noise. The classical approach to learning the variance is via the maximum likelihood estimator – a non-convex optimization problem prone to local minima and with no finite sample complexity bounds. In this paper we study the global system operator: the operator that maps the noises vectors to the output. In particular, we obtain estimates on its spectrum, and as a result derive the first known variance estimators with sample complexity guarantees for online regression problems. We demonstrate the approach on a number of synthetic and real-world benchmarks.

1 Introduction

An online linear regression, or non-stationary regression, is a situation where we are given a sequence of scalar observations \( \{Y_t\}_{t \leq T} \subset \mathbb{R} \), and observation vectors \( \{u_t\}_{t \leq T} \subset \mathbb{R}^n \) such that \( Y_t = \langle X_t, u_t \rangle + z_t \) where \( X_t \in \mathbb{R}^n \) is a regressor vector, and \( z_t \) a random noise term. In contrast to a standard linear regression, the vector \( X_t \) may change with time. Our objective is at time \( T \) to forecast \( Y_{T+1} \) and provide an estimate of \( X_T \), given all previous observation vectors and observations, \( \{u_t\}_{t \leq T}, \{Y_t\}_{t \leq T} \), and the observation vector \( u_{T+1} \).

In this paper we model the problem as follows:

\[
X_{t+1} = X_t + h_t \tag{1}
\]
\[
Y_t = \langle X_t, u_t \rangle + z_t \tag{2}
\]

where \( z_t, h_t \) are zero mean Gaussian random variables, such that \( z_t \) have variance \( \eta^2 \), \( z_t \sim N(0, \eta^2) \) and \( h_t \) take values in \( \mathbb{R}^n \), have a diagonal covariance and
variance $\sigma^2$, $h_t \sim N(0,\sigma^2 I)$. The process noise $h_t$ and the observation noise $z_t$ are assumed to be independent. The vectors $u_t$ are an arbitrary sequence in $\mathbb{R}^n$, such that $u_{t+1}$ is always known to us at time $t$.

The system (1)-(2) is a special case of a Linear Dynamical System (LDS). As is well known, when the parameters $\sigma, \eta$ are given, the mean-squared loss optimal forecast for $Y_{T+1}$ and estimate for $X_T$ are obtained by the Kalman Filter (see for instance [Anderson and Moore, 1979] [Hamilton, 1994] [Chui and Chen, 2017]). In this paper we are concerned with estimators for $\sigma, \eta$, and sample complexity guarantees for these estimators.

Before we discuss the problem in more detail, let us make a few remarks on the special place of the system (1)-(2) among general LDSs. A general LDS may allow the hidden state $X_t$ to evolve in a more complex way, $X_{t+1} = AX_t + h_t$, for some linear operator $A : \mathbb{R}^n \to \mathbb{R}^n$. However, if we do not have any reason to believe that the evolution of $X_t$ is governed by some, especially linear, regularity, then $A = I$, the form in (1), is appropriate. Moreover, in that form, one may regard the problem of estimating $\sigma, \eta$ in (1)-(2) as a pure case of finding the optimal learning rate for $X_t$. Indeed, by inspecting the Kalman filter equations, one easily sees that the effect of $\sigma$ and $\eta$ is to balance how much the estimate for $X_{T+1}$ is influenced by the most recent observation compared to the previous once, which are encoded as the current state $X_T$. Roughly speaking, as shown in Figure 1 higher values of $\sigma$ or lower values of $\eta$ would imply that the past observations are given less weight, and result in an overfit of the forecast to the most recent observation. On the other hand, very low $\sigma$ or high $\eta$ would make the problem similar to the standard linear regression, where all observations are given equal weight, and result in a lag of the forecast.

Let us give an example of a situation where the system (1)-(2) may be used. The Auto-regressive (AR) models [Hamilton, 1994] are perhaps the most widely used time series models. We note that if we take (1)-(2) with constant $X_t$ and choose $u_{T+1} = (Y_T, Y_{T-1}, \ldots, Y_{T-n})$, then we obtain the standard AR($n$) model of the data. It therefore follows that (1)-(2) may model in particular an extension of an AR($n$) time series, where the AR coefficients are no longer restricted to be constant.

We now discuss the problem of estimating $\sigma$ and $\eta$. Note that the standard method of learning the LDS parameters in general, is by finding the parameters that maximize the data likelihood function [Hamilton, 1994] [Anderson and Moore, 1979] [Shumway and Stoffer, 2011]. While the maximum likelihood estimator itself has asymptotic consistency guarantees, the optimization problem of finding the optimal parameters is non-convex and is known to be prone to local maxima issues. In addition, there is a significant amount of classical and ongoing work on forecasting and estimation guarantees for a variety of types of LDSs. However, as we discuss in more detail in Section 2, none of these results apply in the setting of the system (1)-(2), and, arguably, address aspects of the problem that are very different from the main issues that the system (1)-(2) presents. For instance, the Subspace Identification methods [van Overschee and de Moor, 1996] apply only in the stationary setting. The improper learning methods such as [Anava et al., 2013] [Liu et al., 2016] [Kozdoba et al., 2019] apply only when the
Kalman gain (or a related quantity) converges, while the improper learning methods such as [Hazan et al., 2017], are designed for systems that are mainly driven by inputs, and do not address the process noise. In this work we introduce an estimation algorithm for $\sigma, \eta$, termed STVE (Spectrum Thresholding Variance Estimator), and prove finite sample complexity bounds for it, which are the first performance guarantees for the system (1)-(2).

The rest of the paper is organized as follows: In Section 2 we discuss the related work. In Section 3 we introduce the STVE algorithm, state its main guarantees (Theorem 1) and describe in general lines the arguments required to obtain the guarantees. Due to the space constraints, the full details are given in the proof of Theorem 1 in the Supplementary Material Section A. The main theoretical statements are given in Section 4 and proved in the Supplementary Material. In Section 5 we present experimental results on synthetic and real data, and conclusions and future work are discussed in Section 6.

2 Literature

We refer to [Chui and Chen, 2017, Hamilton, 1994, Anderson and Moore, 1979, Shumway and Stoffer, 2011] for a general background on LDSs, the Kalman Filter and maximum likelihood estimation.

The Subspace Identification methods [van Overschee and de Moor, 1996] are a well known alternative approach to the maximum likelihood estimation of LDS system parameters. However, these methods are only applicable if the system is stationary, in the sense that the distribution of the hidden state $X_t$ is time-invariant, and in addition if the observation vectors $u_t$ are constant, independent of $t$.

Another alternative to the maximum likelihood estimation is the improper learning setting, where one provides forecasts of a linear dynamical system from past observations without directly learning the system parameters. This
is done by finding an approximation of the system within a possibly larger, yet simpler, set of models. In particular \cite{Anava et al., 2013, Liu et al., 2016, Kozdoba et al., 2019} provide results along these lines for ARMA, ARIMA, and a general subset of LDSs, respectively. As in the case of Subspace Identification, these results rely heavily on the fact that the observation transformation is constant. Indeed, the case where the observation transformation is constant is principally different from the time varying case. In the former case, the Kalman gain converges, thus yielding asymptotic invariance properties, while in the later, the Kalman gain depends on the sequence $u_t$ and does not need to converge. Another line of research via the improper learning approach studies the dependence of the system on the inputs \cite{Hazan et al., 2017, Hazan et al., 2018}. However, these approaches do not provide forecasting bounds for systems such as (1)-(2).

3 Overview of the approach

We begin by rewriting (1)-(2) in a vector form. To this end, we first encode sequences of $T$ vectors in $\mathbb{R}^n$, \{$a_t\}_{t \leq T} \subset \mathbb{R}^n$, as a vector $a \in \mathbb{R}^{Tn}$, constructed by concatenation of $a_t$'s. Next, we define the summation operator $S' : \mathbb{R}^T \rightarrow \mathbb{R}^T$ which acts on any vector $(h_1, h_2, \ldots, h_T) \in \mathbb{R}^T$ by

$$S'(h_1, h_2, \ldots, h_T) = (h_1, h_1 + h_2, \ldots, \sum_{i \leq t-1} h_i, \sum_{i \leq T} h_i). \quad (3)$$

Note that $S'$ is an invertible operator. Next, we similarly define the summation operator $S : \mathbb{R}^{Tn} \rightarrow \mathbb{R}^{Tn}$, an $n$-dimensional extension of $S'$, which sums $n$-dimensional vectors. Formally, for $(h_i)_{i=1}^{Tn} \in \mathbb{R}^{Tn}$, and for $1 \leq j \leq n, 1 \leq t \leq T$, $(Sh)_j^{(t-1)n+j} = \sum_{i \leq t} h_i^{(t-1)n+j}$. Observe that if the sequence of process noise terms $\beta_1, \ldots, \beta_T \in \mathbb{R}^n$ is viewed as a vector $\beta \in \mathbb{R}^{Tn}$, then by definition $S\beta$ is the $\mathbb{R}^{Tn}$ encoding of the sequence $X_t$.

Next, given a sequence of observation vectors $u_1, \ldots, u_T \in \mathbb{R}^n$, we define the observation operator $O_u : \mathbb{R}^{Tn} \rightarrow \mathbb{R}^T$ by $(O_u h)_t = \langle u_t, \{h_{(t-1)n+1}, \ldots, h_{(t-1)n+n}\}\rangle$. In words, coordinate $t$ of $O_u h$ is the inner product between $u_t$ and $t$-th part of the vector $h \in \mathbb{R}^{Tn}$. With this notation, and also define $Y \in \mathbb{R}^T$ to be the concatenation of $Y_1, \ldots, Y_T$, one may equivalently rewrite the system (1)-(2) as follows:

$$Y = O_u Sh + z, \quad (4)$$

where $h \sim N(0, \sigma^2 I)$ and $z \sim N(0, \eta^2 I)$ are Gaussians in $\mathbb{R}^{Tn}$ and $\mathbb{R}^T$ respectively.

Up to now, we have reformulated our data model as a single vector equation. Note that in that equation, the observations $Y$ and both operators $O_u$ and $S$ are

\footnote{This implicitly assumes that the initial value, $X_1$, is distributed as $N(0, \sigma^2 I)$. We keep this assumption throughout the paper for the simplicity of the notation. As shown in Remark this does not affect the generality of the results.}
known to us. Our problem may now be reformulated as follows: Given $Y \in \mathbb{R}^T$, assuming $Y$ was generated by (4), provide estimates of $\sigma, \eta$.

As a first step of our approach, let $O_u S : \mathbb{R}^T \rightarrow \mathbb{R}^{Tn}$ be the pseudo-inverse, or Moore-Penrose inverse of $O_u S$. Specifically, let

$$O_u S = U \circ \text{Diag}(\gamma_1, \ldots, \gamma_T) \circ W,$$

be the singular value decomposition of $O_u S$, where $\gamma_1 \geq \gamma_2 \geq \ldots \geq \gamma_T > 0$ are the singular values. We assume for the rest of the paper that all of the observation vectors $u_t$ are non-zero. We discuss this assumption, and the extent to which it may be avoided, later in this section. Under this assumption, since $S$ is invertible, $O_u S$ has exactly $T$ non-zero singular values. For $i \leq T$, denote $\chi_i = \gamma_{i+1} - 1 - \gamma_i$. Then $\chi_i$ are the singular values of $R$, arranged in a non-increasing order, and we have by definition

$$R = W^* \circ \text{Diag}(\chi_T, \chi_{T-1}, \ldots, \chi_2, \chi_1) \circ U^*.$$  

To see how one might proceed towards estimating $\sigma$ and $\eta$, consider the expectation of $\|RY\|^2$ with respect to $h, z$, where $|·|$ is the Euclidean vector norm. We have $E|RY|^2 = \|RO_u S\|^2_{HS} \sigma^2 + \|R\|^2_{HS} \eta^2$. Here $\|\|_{HS}$ denotes the Hilbert-Schmidt norm (also known as Frobenius norm, as defined in (17)) of an operator. From the definitions (5), (6), we have that all $T$ singular values of $RO_u S$ are 1 and hence $\|RO_u S\|^2_{HS} = T$. Therefore

$$\frac{E|RY|^2}{T} = \sigma^2 + \frac{\|R\|^2_{HS}}{T} \eta^2.$$  

It follows that if we knew $E|RY|^2$ then we would have one linear relation between two unknowns, $\sigma^2$ and $\eta^2$. Since we only have a realization of $|RY|^2$ rather than the expectation, it follows from the standard measure concentration arguments that if $\sqrt{\frac{\text{Var}|RY|^2}{T}}$ is $o(1)$ as $T$ grows, then we may replace the expectation by $|RY|^2$. This is done in Section 4.

Next, we would like to obtain another, different linear relation between $\sigma^2$, $\eta^2$. To this end, we replace $R$ by a different operator. Set

$$p = \min \left\{ l \geq 1 \mid \sum_{i=1}^{l} \chi_i^2 \geq \frac{1}{2} \|R\|^2_{HS} \right\}.$$  

Thus $p$ is the first index such that the sum of squares of the singular values of $R$ up to $p$ is at least half of the sum of all squares. We define $R' : \mathbb{R}^T \rightarrow \mathbb{R}^{Tn}$ to be a version of $R$ truncated to the first $p$ singular values. If (6) is the SVD decomposition of $R$, then

$$R' = W^* \circ \text{Diag}(0, \ldots, 0, \chi_p, \chi_{p-1}, \ldots, \chi_1) \circ U^*.$$  

Similarly to the case for $R$, we have

$$\frac{E|R'Y|^2}{p} = \sigma^2 + \frac{\|R'\|^2_{HS}}{p} \eta^2,$$
Algorithm 1 Spectrum Thresholding Variance Estimator (STVE)

1: **Input:** Observations $Y_t$, observation vectors $u_t$, with $t \leq T$.
2: Compute the SVD of $O_u S$,

$$O_u S = U \circ \text{Diag}(\gamma_1, \ldots, \gamma_T) \circ W,$$

where $\gamma_1 \geq \gamma_2 \geq \ldots \geq \gamma_T > 0$. Denote $\chi_i = \gamma_{T+1-i}^{-1}$ for $1 \leq i \leq T$.
3: Set

$$p = \min \left\{ l \geq 1 \mid \sum_{i=1}^{l} \chi_i^2 \geq \frac{1}{2} \sum_{i=1}^{T} \chi_i^2 \right\}.$$
4: Construct the operators

$$R = W^* \circ \text{Diag}(\chi_T, \ldots, \chi_1) \circ U^*$$
and

$$R' = W^* \circ \text{Diag}(0, \ldots, 0, \chi_p, \ldots, \chi_1) \circ U^*$$
5: Produce the estimates:

$$\hat{\eta}^2 = \left( \frac{|R'Y|^2}{p} - \frac{|RY|^2}{T} \right) \left( \frac{\|R'\|_{HS}^2}{p} - \frac{\|R\|_{HS}^2}{T} \right)^{-1},$$

$$\hat{\sigma}^2 = \frac{|RY|^2}{T} - \frac{\|R\|_{HS}^2}{T} \hat{\eta}^2.$$

and appropriate concentration arguments ensure that one may replace the expectation $E |R'Y|^2$ by the realization $|R'Y|^2$. Finally, given the relations (7) and (9), one may solve the system to obtain estimates for $\hat{\sigma}^2, \hat{\eta}^2$. The procedure is summarized as Algorithm 1.

Our main theoretical result provides error bounds for the estimators $\hat{\sigma}^2, \hat{\eta}^2$ calculated by Algorithm 1.

**Theorem 1.** Consider a random vector $Y \in \mathbb{R}^T$ of the form $Y = O_u Sh + z$ where $h \sim N(0, \sigma^2 I)$ in $\mathbb{R}^T_n$ and $z \sim N(0, \eta^2 I)$ in $\mathbb{R}^T$. Define $|u_{\max}| = \max_t |u_t|$ and $|u_{\min}| = \min_t |u_t|$. Then for every $0 < \varepsilon < \frac{1}{2}$, for every $T > 0$, with probability at least $1 - 6T^{-2\varepsilon}$ the estimators $\hat{\sigma}^2$ and $\hat{\eta}^2$ satisfy:

$$|\eta^2 - \hat{\eta}^2| \leq c \frac{1}{T^{1-\varepsilon}} \frac{|u_{\max}| \log T}{|u_{\min}|^3} \left( \frac{\|R'\|_{HS}^2}{p} - \frac{\|R\|_{HS}^2}{T} \right)^{-1},$$

$$|\sigma^2 - \hat{\sigma}^2| \leq c \frac{1}{T^{1-\varepsilon}} \left( \frac{1}{|u_{\min}|^2} + \frac{|u_{\max}| \log T}{|u_{\min}|^5} \left( \frac{\|R'\|_{HS}^2}{p} - \frac{\|R\|_{HS}^2}{T} \right)^{-1} \right).$$

Here $c > 0$ is an absolute constant, independent of $T, n, \varepsilon, \sigma, \eta$.

In what follows we first briefly discuss the main ideas underlying the proof of Theorem 1. As noted above, to replace expectations by the samples values, we...
need upper bounds on the expressions $\frac{\sqrt{\text{Var}[R'_Y]^2}}{T}$ and $\frac{\sqrt{\text{Var}[R'_Y]^2}}{p}$. Similarly to the expectations, these quantities can be expressed in terms of the spectrum of the operators $R, R'$. To provide bounds on these spectra, first it will be shown that there are analytical expressions for the spectrum of the operator $S$, which is roughly uniform in the interval $[1, T]$. However, the spectra of the composition $O_u S$ and its inverse $R$ are harder to bound. In particular, in the main technical results of this paper, Lemma 2 and Proposition 3 we bound the nuclear norm of $O_u S$ and use this to show that $R$ has many (order of at least $T/\log T$) singular values $\chi_i$ of constant order. This is then used to show a key fact that $p$, defined in (8), is of order at least $T/\log T$. This in turn leads to upper bounds on the expression $\frac{\sqrt{\text{Var}[R'_Y]^2}}{p}$.

We now take a closer look at the parameters appearing in the bounds (11), (12). First note that some form of lower bound on the norms of the observation vectors $u_t$ must appear in the bounds. This is simply because if one had $u_t = 0$ for all $T$, then clearly no estimate on $\sigma, \eta$ would have been possible. On the other hand, our use of the smallest value $|u_{\text{min}}|$ may seem restrictive at first. This seems to exclude scenarios with missing observations, which are equivalent to $u_t = 0$, and may indicate that small non-zero outlier $u_t$ influences the estimates. To see that this is not the case, we note that one may simply replace the full observation operator $O_u : \mathbb{R}^{Tn} \rightarrow \mathbb{R}^T$ with $O_u : \mathbb{R}^{Tn} \rightarrow \mathbb{R}^T$ that does not use the zero or small-norm observation vector. Theorem 1 will remain unchanged, except that $T$ will be replaced with $\bar{T}$, the actual number of observations used.

Next, the most interesting quantity in the bounds (11), (12) is the term $\frac{\|R'_p\|_{HS}^2}{p} - \frac{\|R\|_{HS}^2}{T}$. This term is the difference between the coefficients of $\eta^2$ in equations (7) and (9), and large values of this term guarantees that these equations are not in fact the same equation twice. For the bounds (11), (12) to be meaningful, we should have roughly

$$\frac{\|R'_p\|_{HS}^2}{p} - \frac{\|R\|_{HS}^2}{T} \geq \frac{1}{T^{\frac{1}{2} + \varepsilon}}. \tag{13}$$

To better understand the quantity $\frac{\|R'_p\|_{HS}^2}{p} - \frac{\|R\|_{HS}^2}{T}$, first note that by definition we have

$$\frac{\|R'_p\|_{HS}^2}{p} \geq \frac{\|R\|_{HS}^2}{T}. \tag{14}$$

In addition, by Proposition 4 (see below), both $\frac{\|R'_p\|_{HS}^2}{p}$ and $\frac{\|R\|_{HS}^2}{T}$ are of order at least $\frac{1}{\log^2 T}$. Therefore, both terms are of much higher order than the lower bound on the difference that we require in (13). Next, note that equality in (14) is obtained only when $\chi_i$ are all the same value. Therefore, the difference in (13) measures how non-constant the spectrum of $R$ is. To gain an intuition as to why the spectrum should be non-constant, we observe that the singular values...
of \((S')^{-1}\), with \(S'\) as defined in \((3)\), satisfy
\[
\lambda_l((S')^{-1}) = \frac{1}{2} \sin^{-1}\left(\frac{\pi l}{2T}\right) \text{ for } l \leq T,
\]
and thus vary continuously from 1 to 0. This is shown in the proof of Lemma \(2\) below. The singular values of \(S'^{-1}\) are \(\lambda_l((S')^{-1})\), each taken with multiplicity \(n\). Since \(R\) is obtained by inverting the composition of \(S\) with \(O_u\), the question of whether \((13)\) holds amounts to whether the composition with \(O_u\) can flatten the non-constant spectrum of \(S\).

In practical terms, however, note that \(R\) is known, and the condition \((13)\) can simply be verified before using the estimator. We suggest the following rule of thumb: check the condition
\[
\frac{\|R'\|_{HS}^2}{p} - \frac{\|R\|_{HS}^2}{T} \geq \frac{1}{10} \frac{\|R\|_{HS}^2}{T}.
\]
(15)
If the condition holds then compute the estimates \(\hat{\sigma}^2, \hat{\eta}^2\). By Proposition \(4\) below we have \(\frac{\|R'\|_{HS}^2}{p} \geq \frac{1}{8 n^2 |u_{\max}|^p \log T} T\). Therefore for sequences \(u_t\) which satisfy \((15)\), the bounds in Theorem \(1\) hold with errors of order at most \(O\left(\frac{1}{T^{1/2}}\right)\), up to logarithmic terms in \(T\). Note that \((15)\) is much stronger than inequality \((13)\), which is sufficient for the errors to be \(o(1)\) in \(T\). Note also that \((13)\) can be equivalently reformulated as
\[
T - p \geq \text{const} \cdot T.
\]
(16)
Nevertheless, \((16)\) seems to hold in practice as we demonstrate on a few datasets in Section \(5\).

4 Properties of \(O_u S\) and \(R\)

In this section we state the key properties of the operators \(O_u S\) and \(R\) as discussed in Section \(3\). The proofs are given in Supplementary Material Sections \(B\) and \(C\).

Let \(A : \mathbb{R}^n \to \mathbb{R}^m\) be an operator with a singular value decomposition \(A = U \circ \text{Diag}(\lambda_1, \ldots, \lambda_s) \circ W\), where \(s \leq \min\{m, n\}\) and \(\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_s > 0\). The Hilbert-Schmidt (Frobenius), nuclear and operator norms are defined, respectively, as
\[
\|A\|_{HS} = \sqrt{\sum_{i=1}^{s} \lambda_i^2}, \quad \|A\|_{nuc} = \sum_{i=1}^{s} \lambda_i, \quad \|A\|_{op} = \lambda_1.
\]
(17)

Lemma 2. Denote by \(\gamma_i\), \(i \leq T\), the singular values of \(O_u S\), arranged in non-increasing order. Then \(O_u S\) is upper and lower bounded by:
\[
\gamma_1 \leq |u_{\max}| T \text{ and } \gamma_T \geq \frac{1}{2} |u_{\min}|.
\]
(18)
Moreover, the nuclear norm of $O_uS$ satisfies

$$
\|O_uS\|_{\text{nuc}} = \sum_{t \leq T} \gamma_i \leq 4n |u_{\text{max}}| T \log T.
$$

(19)

The proof of this lemma uses the following auxiliary result: Let $D_T : \mathbb{R}^T \rightarrow \mathbb{R}^{T-1}$ be the difference operator, $(D_Tx)_t = X_{t+1} - X_t$ for $t \leq T - 1$. The operator $D_T$ has $T - 1$ distinct non-zero singular values as follows:

**Lemma 3.** The operator $D_T$ has kernel of dimension 1 and singular values $\kappa_l(D_T) = 2 \sin \left( \frac{\pi l}{2T} \right)$ for $l = 1, \ldots, T - 1$.

This result is known. In the field of Finite Difference methods, the operator $DD^*$ is known as the discrete second derivative with Dirichlet boundary conditions. The eigenvalues of $DD^*$ may be derived by a direct computation, and correspond to the roots of the Chebyshev polynomial of second kind of order $T$. We refer to [Mitchell and Griffiths, 1980], p.50, for the full proof of Lemma 3.

The following is the key technical result of this paper:

**Proposition 4.** Let $R : \mathbb{R}^T \rightarrow \mathbb{R}^{Tn}$ be the pseudoinverse of $O_uS$. Then $\|R\|_{\text{op}} \leq \frac{2}{|u_{\text{min}}|^{-1}}$ and $\|R\|_{\text{HS}} \geq \frac{1}{8n^2 |u_{\text{max}}|^2 \log^2 T}$.

**Remark 5.** As mentioned in the Introduction, the initial value $X_1$ does not affect the estimates, as long as its norm is of constant order. To see this, note that by definition, $RO_uS$ is an orthogonal projection operator onto the complement of its kernel. Thus, consider any fixed $X_1$, as a vector in $\mathbb{R}^{Tn}$, supported on the first $n$ coordinates. Then we have $|RO_uSX_1| \leq |X_1|$, independent of $T$, while $|RO_uSh|$ is of order $\sqrt{T}$. Similar consideration holds also when $X_1$ is arbitrarily distributed with bounded mean and variance.

## 5 Experiments

In this section we empirically evaluate the STVE algorithm. First, in Section 5.1 we illustrate the spectral properties of the operator $R$ and show that the condition (16) holds in practice. Then, in Section 5.2 we demonstrate the usefulness of our algorithm in online regression. Additional experiments in Supplementary Material Section E compare the variances estimation errors of STVE to EM (ExpectationMaximization), which is a widely used maximum likelihood estimator.

For the EM method and Kalman filter implementation we employ the pykalman package available online[2]. Both our method and pykalman are written in python. All our plots are best viewed in color and our code will be made available online.

[2]https://pykalman.github.io/
Figure 2: Top row: The values of $\chi^2_i$ of $R$. Bottom row: Cumulative sum of $\chi^2_i$ (blue), the linear envelope (orange), and the value of $p$ (green). Columns: left - random data, middle - Dow Jones data, right - energy forecasting data.

Figure 3: Left: Covariance matrix for the energy forecasting data ($n = 11$). Middle and right: mean square error for the synthetic (middle) and energy forecasting (right) datasets.
Datasets  We generated synthetic data by the LDS $\sigma^2 = 1, \eta^2 = 9, n = 5$. The values of $u_t$ where sampled from $N(0, I)$, and truncated to satisfy $1 \leq |u_t| \leq 5$. We also used two real-world datasets. The first is Dow Jones index time series with AR(10) model. The second dataset that we employ is taken from the Kaggle competition ”Global Energy Forecasting Competition 2012 - Load Forecasting”. This dataset includes hourly electric demand for four and a half years from 20 different geographic regions, and appropriate hourly temperature readings from 11 sensors, which we used as features (observation vectors) $u_t \in \mathbb{R}^{11}$. We use hourly readings for region 1 in this experiment, which constitutes $T = 38069$ data points. We normalize the temperatures to range $[0, 1]$ and predict the logarithm of hourly electric demand increase or decrease.

5.1 Spectral properties of the operator $R$

The top row in Figure 2 shows the spectrum for different datasets, and we verify that indeed it is not constant. The bottom row in Figure 2 shows that (16) holds.

5.2 Online Regression Experiments

We evaluate our method in an online regression scenario. We compare 3 approaches: Kalman filter with STVE variance estimation, Kalman filter with EM variance estimation and the Stochastic Gradient Descent (SGD) algorithm with a constant learning rate. For the learning rate of SGD we perform grid search in \{10^{-6}, 5 \cdot 10^{-6}, 10^{-5}, 5 \cdot 10^{-5}, 10^{-4}, 5 \cdot 10^{-4}, 10^{-3}, 5 \cdot 10^{-3}, 10^{-2}, 5 \cdot 10^{-2}, 10^{-1}, 5 \cdot 10^{-1}, 1\}.

First we use the synthetic data with $T = 10000$. We employ 20% of the data to estimate the noise parameters by STVE and EM, and select the learning rate for SGD. We then compare the algorithms on the rest of the data. We run 20 iterations of EM and its runtime was $\sim 50\%$ more than of STVE. We repeat the simulation 40 times and the error bars in the plot correspond to the 95% confidence interval over the 40 runs. The MSE results appear in Fig. 3b. The 'Accurate' line in the plot corresponds to run of Kalman filter with exact (known) variances that generate the data.

We observe that STVE achieves MSE very close to 'Accurate', and outperforms EM. Both outperform the SGD method.

Next we employ the real energy forecasting data. We employ 5% of the data to estimate the noise parameters by STVE and EM, and select the learning rate for SGD. We then compare the algorithms on the rest of the data. We run 25 iterations of EM, and its runtime was similar to STVE ($\sim 35$ seconds).

In Fig. 3a we illustrate the covariance matrix estimated by the EM algorithm. It can be seen that the covariance matrix is not diagonal. Although our approach is limited to diagonal covariance we show that it works very well in

\footnotesize{See http://www.kaggle.com/c/global-energy-forecasting-competition-2012-load-forecasting}
practice. Indeed, in Fig. 3c we compare the MSE of different algorithms and conclude that our approach STVE outperforms other competitors.

6 Conclusion and Future Work

In this work we introduced the STVE algorithm for estimating the variance parameters of LDSs of type (1)-(2), and obtained sample complexity guarantees for the estimators.

We now briefly discuss possible extensions of this work to more general LDSs. An extension to vector rather than scalar valued observations is straightforward, and can be done along the line of the current argument, with virtually no changes in the analysis of the operator $O_u$. The extension to the case where the dynamics of $X$ is governed by an equation of the form $X_{t+1} = AX_t + h_t$, even if $A \neq I$ is known, is more delicate. On one hand, the analysis of the spectrum of the corresponding operator $S$ would require new ideas. However, on the other hand, the operator $S$ contains all the information about the behavior of the hidden state, and therefore a systematic study of its spectrum should provide us with a clearer understanding of the temporal properties of the system.

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A Proof of Theorem 1

Proof. We use the notation introduced in Section 1. Throughout the proof, fix some \( 0 < \varepsilon < \frac{1}{2} \), which will serve as the tradeoff between the probability bounds and the size of the error term.

Note that since \( S \) is invertible and \( O_u \) has rank \( T \), the operator \( R O_u S \) has a single eigenvalue 1, with multiplicity \( T \). In particular, \( \| R O_u S \|_{HS}^2 = T \).

Similarly, we have \( \| R' O_u S \|_{HS}^2 = p \).

We first consider the expressions

\[
|RY| = |R O_u S h + R z| \quad \text{and} \quad |R' Y| = |R' O_u S h + R' z|.
\]

By Lemma 8 in Section D (applied with \( A = R O_u S \) and \( B = R' \)), we have

\[
\frac{|RY|}{T} = \sigma^2 + \frac{\| R \|_{HS}^2}{T} \eta^2 + O \left( T^{\varepsilon} \left( \frac{\sqrt{T}}{T} + \frac{\| R^* R \|_{HS}}{T} + \frac{\| R^* R O_u S \|_{HS}}{T} \right) \right).
\]

(20)

Similarly for \( R' \),

\[
\frac{|R' Y|}{p} = \sigma^2 + \frac{\| R' \|_{HS}^2}{p} \eta^2 + O \left( p^{\varepsilon} \left( \frac{\sqrt{p}}{p} + \frac{\| R'^* R' \|_{HS}}{p} + \frac{\| R'^* R' O_u S \|_{HS}}{p} \right) \right).
\]

(21)

We begin by bounding the error terms in the main equations, (20) and (21).

Specifically, we show that

\[
\left( \frac{\sqrt{T}}{T} + \frac{\| R^* R \|_{HS}}{T} + \frac{\| R^* R O_u S \|_{HS}}{T} \right) \leq T^{-\frac{1}{2}} \left( 1 + \frac{4}{|u_{\min}|^2} + \frac{2}{|u_{\min}|} \right) \leq c \frac{T^{-\frac{1}{2}}}{|u_{\min}|^2},
\]

(22)

and

\[
\left( \frac{\sqrt{p}}{p} + \frac{\| R'^* R' \|_{HS}}{p} + \frac{\| R'^* R' O_u S \|_{HS}}{p} \right) \leq p^{-\frac{1}{2}} \left( 1 + \frac{4}{|u_{\min}|^2} + \frac{2}{|u_{\min}|} \right) \leq cT^{-\frac{1}{2}} \frac{\log T}{|u_{\min}|^3}.
\]

(23)

To show (22), first observe that

\[
\| R^* R \|_{HS} = \sqrt{\sum_{i \leq T} \chi_i^4} \leq \sqrt{T} \left( \max_{i \leq T} \chi_i \right)^2 = \sqrt{T} \| R \|_{op}^2 \leq 4\sqrt{T}. \]

(24)
where the last inequality follows from Proposition 4. Next, since \(RO_uS\) is an orthogonal projection operator onto the image of \(R\), the spectrum of \(R^*RO_uS\) is identical to the spectrum of \(R^*\) and we have

\[
\|R^*RO_uS\|_{HS} = \|R^*\|_{HS} = \|R\|_{HS} \leq \sqrt{T} \|R\|_{op} \leq \frac{2\sqrt{T}}{|u_{min}|}.
\]  

(25)

Combining (24) and (25) yields the first inequality in (22), while the second one follows trivially. Next, to obtain (23), first note that by Proposition 4, we have

\[
\chi_1^2 = \max_i \chi_i^2 \leq 4|u_{min}|^{-2} \quad \text{and} \quad \sum_{i \leq T} \chi_i^2 \geq \frac{1}{8n^2 |u_{max}|^2} \log^2 T.
\]  

(26)

These equations imply that since the sum \(\sum_{i \leq T} \chi_i^2\) is of order \(T\), while all the summands are of constant order, it follows that \(p\), defined in (8), must be of order \(T\). Specifically, we have

\[
p \geq \frac{1}{2} \cdot \frac{1}{8n^2 |u_{max}|^2} \log^2 T \cdot \left(4|u_{min}|^{-2}\right)^{-1} = \frac{|u_{min}|^2}{64n^2 |u_{max}|^2} \log^2 T.
\]  

(27)

Next, we clearly have \(\|R\|_{op} = \|R^*\|_{op}\). Therefore similarly to the argument for \(R\), we obtain

\[
\|R^*R\|_{HS} = \frac{4\sqrt{p}}{|u_{min}|^2} \quad \text{and} \quad \|R^*RO_uS\|_{HS} = \frac{2\sqrt{p}}{|u_{min}|}.
\]  

(28)

The inequality (23) follows by combining (27) and (28). Finally, by Lemma 8 each of the inequalities (20) and (21) holds with probability at least \(1 - 3T^{-2\epsilon}\). Therefore both of them together hold with probability at least \(1 - 6T^{-2\epsilon}\). The inequality (11) is obtained by subtracting (20) from (21) and using (22),(23). The inequality (12) follows in turn from (20) and (11), and by observing again that \(\frac{\|R\|_{op}}{\sqrt{T}} \leq \frac{4}{|u_{min}|^2}\). \(\square\)

B Proof of Lemma 2

Proof. We first establish the bounds on the spectrum of \(S\). To this end, denote by \(S'_T\) the version of \(S\) with \(n = 1\). Then one may readily check that the operator \(D_T \circ S'_T : \mathbb{R}^T \rightarrow \mathbb{R}^{T-1}\) satisfies

\[
D_T S'_T(x_1, x_2, \ldots, x_T) = (x_2, \ldots, x_T).
\]  

(29)

Thus \(D_T\) is almost an inverse of \(S'_T\). This fact, in conjunction with the special form of \(S'_T\), allows to derive the spectral properties of \(S'_T\) from those of \(D\). We now proceed to show this. Denote by \(V_1 \subset \mathbb{R}^T\) the space spanned by all except the first coordinates in \(\mathbb{R}^T\), \(V_1 = \text{span}\{e_2, \ldots, e_T\}\) where \(e_i\) are the standard basis in \(\mathbb{R}^T\). Then (29) implies that \(DS'_T\) restricted to \(V_1\) is an
identity. Therefore, the singular values of $S'$ restricted to $V_1$ are precisely $\kappa_l^{-1}$, for $l = 1, \ldots, T - 1$. To connect the singular values of $S'_T$ to the those of $S'_T$ restricted to $V_1$, it remains to observe that $V_1$ is an invariant subspace of $S'_T$, and that the action of $S'_T$ on $V_1$ is unitarily equivalent to the action of $S'_T^{-1}$ on $\mathbb{R}^{T-1}$. Combining these two observations, we obtain that the singular values of $S'_T$ are $\kappa_l^{-1}(T + 1)$, for $l = 1, \ldots, T$, i.e. the inverse singular values of $D_{T+1}$.

In particular, using the inequality

$$\sin \frac{\pi}{2} \alpha \geq \alpha \text{ for all } \alpha \in [0, 1],$$

it follows that for all $x \in \mathbb{R}^T$,

$$|S'_T x|^2 \leq \frac{1}{4 \sin^2 \left( \frac{\pi}{2(T+1)} \right)} |x|^2 \leq \frac{1}{4} (T + 1)^2 |x|^2$$

and

$$|S'_T x|^2 \geq \frac{1}{4} |x|^2.$$

Note also that $S$ is by definition a collection of $n$ independent copies of $S'_T$, and therefore the spectrum of $S$ is that of $S'_T$, but each singular value is taken with multiplicity $n$. In particular it follows that (31) and (32) hold also for $S$ itself.

Next, note that since $O_u$ mixes the different copies of $S'_T$ in $S$, it does not seem possible to obtain a direct expression for the spectrum of $O_u S$. However, we can still control the upper and lower bounds. To obtain the upper bound, note that we clearly have the operator norm bound for $O_u$:

$$|O_u x| \leq |u_{\max}| |x|.$$  

Combining (33) and (34), we obtain the upper bound in (18).

For the lower bound, denote by $V'$ the orthogonal complement to the kernel of $O_u$, $V' = (\text{Ker}(O_u))^\perp$. Denote by $P_{V'} : \mathbb{R}^{Tn} \rightarrow V'$ the orthogonal projection onto $V'$. We have in particular that $O_u S = O_u P_{V'} S$. Next, the operator $S$ maps the unit ball $B_{Tn}$ of $\mathbb{R}^{Tn}$ into an ellipsoid $E_T$, and by (32), we have $\frac{1}{2} B_{Tn} \subset E_T$. It therefore follows that

$$\frac{1}{2} B_{V_1} \subset (P_{V'} S)(B_{Tn}),$$

where $B_{V_1}$ is the unit ball of $V_1$. It remains to observe that for every $x \in V_1$, we have

$$|O_u x| \geq |u_{\min}| |x|.$$  

Combining (34) and (35), we obtain the lower bound in (18).

Finally, to derive (19), recall that the nuclear norm is sub-multiplicative with respect to the operator norm (see for instance [Gohberg and Krein, 1969], Chapter 2, eq. 2.2 for a much stronger fact). Therefore

$$\|O_u S\|_{\text{nuc}} \leq \|O_u\|_{\text{op}} \cdot \|S\|_{\text{nuc}} \leq |u_{\max}| \cdot \|S\|_{\text{nuc}},$$

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where the second inequality follows from (33). Next, since the spectrum of \( S \) is the spectrum of \( S' \) taken with multiplicity \( n \), we have

\[
\|S\|_{\text{nuc}} = n \|S'\|_{\text{nuc}}. \tag{37}
\]

It remains to bound the nuclear norm of \( S' \). Using (30) again, we have

\[
\|S'\|_{\text{nuc}} = 2 \sum_{t \leq T} \sin^{-1} \left( \frac{\pi t}{2(T+1)} \right) \leq 2T \sum_{t \leq T} \frac{1}{t+1} \leq 4T \log T. \tag{38}
\]

Combining (30), (37) and (38), the inequality (19) follows.

C Proof of Proposition 4

Proof. The bound on \( \|R\|_{\text{op}} \) follows directly from the lower bound on the singular values of \( OuS \) in (18). To bound \( \|R\|_{HS} \), note that from (19) in Lemma 2, the number of \( \gamma_i \) that are larger than \( 4n |u_{\max}| \log T \) satisfies

\[
\# \{ \gamma_i \mid \gamma_i \geq 4n |u_{\max}| \log T \} \leq \frac{T}{2}. \tag{39}
\]

Since there are total of \( T \) singular values \( \gamma_i \) overall, we can equivalently rewrite (39) as

\[
\# \left\{ \gamma_i \mid \gamma_i^{-1} \geq \frac{1}{4n |u_{\max}| \log T} \right\} \geq \frac{T}{2}.
\]

This immediately implies the lower bound on \( \|R\|_{HS}^2 \).

D Concentration Bounds Proofs

In this section we state the results required for the concentration arguments. Lemmas 6 and 7 are computations using the singular value decomposition, while Lemma 8 follows directly from Chebyshev inequality, via Lemmas 6, 7 and a union bound.

Lemma 6. Let \( A : \mathbb{R}^n \to \mathbb{R}^m \) be an operator, and \( h \sim N(0, \sigma^2 I) \) a Gaussian vector with diagonal covariance. Denote by \( \{\lambda_i\}_{i=1}^{k}, k \leq \min(m, n), \) the singular values of \( A \). Then

\[
\mathbb{E} |Ah|^2 = \sigma^2 \|A\|_{HS}^2 = \sigma^2 \sum_{i=1}^{k} \lambda_i^2, \tag{40}
\]

and

\[
\text{Var} |Ah|^2 = 2\sigma^4 \|A^*A\|_{HS}^2 = 2\sigma^4 \sum_{i=1}^{k} \lambda_i^4. \tag{41}
\]
Proof. Write $A$ in its singular value decomposition form:

$$A = \sum_{i=1}^{k} \lambda_i \phi_i \otimes \psi_i. \quad (42)$$

Here $\lambda_i$, $1 \leq i \leq k$ are the singular values of $A$, $\psi_i$ are orthogonal vectors in $\mathbb{R}^m$ and $\phi_i$ are orthogonal vectors in $\mathbb{R}^n$. The notation $\phi_i \otimes \psi_i$ denotes an operator $\mathbb{R}^n \to \mathbb{R}^m$ which acts by $\langle \phi_i \otimes \psi_i \rangle v = \langle \phi_i, v \rangle \psi_i$. By the rotational invariance of the Gaussian, we can write

$$h = \sum_{i \leq k} h_i \phi_i, \quad (43)$$

where $h_i$ are i.i.d scalar $N(0, \sigma^2)$ variables. Now,

$$E |Ah|^2 = E \langle Ah, Ah \rangle = E \left( \sum_{i \leq k} \lambda_i h_i \phi_i \otimes \psi_i, \sum_{j \leq k} \lambda_j h_j \phi_j \otimes \psi_j \right) = E \sum_i \lambda_i^2 h_i^2 = \sigma^2 \sum_i \lambda_i^2. \quad (46)$$

Next,

$$Var |Ah|^2 = E \langle Ah, Ah \rangle^2 - \left( E |Ah|^2 \right)^2$$

$$= E \left( \sum_i \lambda_i^2 h_i^2 \right)^2 - \sigma^4 \left( \sum_i \lambda_i^2 \right)^2$$

$$= \left( \sum_{i,j} \lambda_i^2 \lambda_j^2 h_i^2 h_j^2 \right)^2 - \sigma^4 \left( \sum_i \lambda_i^2 \right)^2$$

$$= \left( \sum_{i,j} \lambda_i^2 \lambda_j^2 \mathbb{E} h_i^4 h_j^2 \right) - \sigma^4 \left( \sum_i \lambda_i^2 \right)^2$$

$$= \sum_i \lambda_i^2 \mathbb{E} h_i^4 + \sum_{i \neq j} \lambda_i^2 \lambda_j^2 \sigma^2 - \sigma^4 \left( \sum_i \lambda_i^2 \right)^2. \quad (47)$$

Since for $h_i \sim N(0, \sigma^2)$ we have $\mathbb{E} h_i^4 = 3 \sigma^4$, the equality (41) follows from (47). \qed 

Similarly,
Lemma 7. Let $A : \mathbb{R}^n \to \mathbb{R}^m$ be an operator, and $h \sim N(0, \sigma^2 I)$, $z \sim N(0, \eta^2 I)$ Gaussian vectors in $\mathbb{R}^n$ and $\mathbb{R}^m$ respectively. Denote by $\lambda_i$, $i \leq k$, the singular values of $A$. Then $\mathbb{E} \langle Ah, z \rangle = 0$ and

$$\text{Var} \langle Ah, z \rangle = \mathbb{E} \langle Ah, z \rangle^2 = \sigma^2 \eta^2 \|A\|_{HS}^2 = \sigma^2 \eta^2 \sum_{i=1}^{k} \lambda_i^2.$$

Proof. We have $\mathbb{E} \langle Ah, z \rangle = 0$ due to the independence of $h, z$. Next, similarly to the proof of Lemma 6, write $A = \sum_{i=1}^{k} \lambda_i \phi_i \otimes \psi_i$, $h = \sum_{i \leq k} h_i \phi_i$, $z = \sum_{i \leq k} z_i \psi_i$.

Then

$$\mathbb{E} \langle Ah, z \rangle^2 = \mathbb{E} \left( \sum_{i \leq k} \lambda_i h_i z_i \right)^2 = \mathbb{E} \sum_{i,j \leq k} \lambda_i \lambda_j h_i z_i h_j z_j$$

$$= \mathbb{E} \sum_{i} \lambda_i^2 h_i^2 z_i^2 + \mathbb{E} \sum_{i \neq j} \lambda_i \lambda_j h_i z_i h_j z_j$$

$$= \sum_{i} \lambda_i^2 \mathbb{E} h_i^2 z_i^2 + \mathbb{E} \sum_{i \neq j} \lambda_i \lambda_j \mathbb{E} h_i z_i h_j z_j$$

$$= \sum_{i} \lambda_i^2 \sigma^2 \eta^2 + 0.$$

$Lemmas 8$. Consider a random variable $Y = Ah + Bz$, where $h \sim N(0, \sigma^2 I)$ and $z \sim N(0, \eta^2 I)$ are Gaussian variables in $\mathbb{R}^n_A$ and $\mathbb{R}^n_B$ respectively, and $A : \mathbb{R}^n_A \to \mathbb{R}^m$, $B : \mathbb{R}^n_B \to \mathbb{R}^m$ are linear operators.

Then for any $T > 0$ and $\varepsilon > 0$,

$$\mathbb{P} \left[ \frac{|Y|^2}{\|A\|_{HS}^2} - \left( \frac{\|B\|_{HS}^2}{\|A\|_{HS}^2} \right) \geq T \varepsilon \left( \sigma^2 \frac{\|A^* A\|_{HS}}{\|A\|_{HS}^2} + \eta^2 \frac{\|B^* B\|_{HS}}{\|A\|_{HS}^2} + 2\sigma \eta \frac{\|B^* A\|_{HS}}{\|A\|_{HS}^2} \right) \right] \leq 3 \frac{1}{T^{2 \varepsilon}}.$$

Proof. The results follows directly from Chebyshev inequality, via Lemmas [6] and [7] and a union bound. Indeed, write

$$|Y|^2 = |Ah|^2 + |Bz|^2 + 2 \langle Ah, Bz \rangle$$

$$= |Ah|^2 + |Bz|^2 + 2 \langle B^* Ah, z \rangle.$$

(53)
To each of the terms in (53) we apply the Chebyshev inequality in the following form: For any random variable $X$, any $T > 0$ and $\varepsilon > 0$, 

$$
\mathbb{P}\left( |X - \mathbb{E}X| \geq T\varepsilon \sqrt{\text{Var}X} \right) \leq \frac{1}{T^2\varepsilon^2}.
$$

The expectations and variances of the terms in (53) are given by Lemmas 6 and 7, and the conclusion follows by dividing everything by $\|A\|_{HS}^2$ and using the union bound.

## E Additional experiments

We compare the error in variances estimations of STVE to EM.

We run both estimation methods for 2000 and 4000 data samples from our synthetic data (described in Section 5), and plot the estimation error against runtime of the methods. Note that EM is an iterative algorithm and by changing
the number of iterations we control its runtime and estimation accuracy. Although EM estimates full covariance matrix, it is indeed very close to diagonal matrix, as we illustrate in Figure 5. Therefore, we define the error in variance estimation of EM to be the average of errors between the diagonal values and the true value $\sigma^2 = 1$. We repeat the simulation 5 times and the error bars in the plots correspond to the 95% confidence interval over the 5 runs.

The results appear in Figure 4. We observe that STVE achieves smaller errors for both process noise variance and observation noise variance. In addition, increasing the number of samples ($T$) decrease the errors, as expected.