Data-driven pattern identification and outlier detection in time series

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Abstract—We address the problem of data-driven pattern identification and outlier detection in time series. To this end, we use singular value decomposition (SVD) which is a well-known technique to compute a low-rank approximation for an arbitrary matrix. By recasting the time series as a matrix it becomes possible to use SVD to highlight the underlying patterns and periodicities. This is done without the need for specifying user-defined parameters. From a data mining perspective, this opens up new ways of analyzing time series in a data-driven, bottom-up fashion. However, in order to get correct results, it is important to understand how the SVD-spectrum of a time series is influenced by various characteristics of the underlying signal and noise. In this paper, we have extended the work in earlier papers by initiating a more systematic analysis of these effects. We then illustrate our findings on some real-life data.

Keywords—Data mining; time series; outliers; singular value decomposition (SVD); parameter-free approximation.

I. INTRODUCTION

A. Motivation

Since the gathering of the sensor data has become relatively cheap and straightforward, nowadays it is common to collect detailed information about all sorts of processes and services that take place in factories, infrastructural networks and public spaces. In many of these applications (especially those related to human activities), there is a multitude of time series in which a pronounced but relatively short periodicity (e.g. daily pattern) is superimposed on a slower, more global trend. If we sprinkle a bit of noise onto the time series, the columns in A will no longer be identical, but still very similar. As a consequence, the expression in (1) will still hold to a very good approximation. This observation is the motivation for the introduction of singular value decomposition (SVD) which we will briefly recapitulate below.

B. SVD recapitulation and some notation

The basic result that we will use throughout the paper is the following well-known theorem.

Theorem: Singular Value Decomposition (SVD) Given an arbitrary $p \times q$ matrix $A \in \mathbb{R}^{p \times q}$, then there exists matrices $U$ and $V$ (both with orthonormal columns), and positive numbers $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_r$ (where $r = \min(p,q)$), such that:

$$A = \sum_{k=1}^{r} \sigma_k U_k V_k^T$$

(2)

with $U_k$ and $V_k$ denoting the $k^{th}$ column of $U$ and $V$, respectively, and $S$ is an $p \times q$ matrix for which the numbers $\sigma_k$ (the singular values) are placed on the main diagonal. For a proof, see e.g. [4].

In the remainder of this paper, we will assume that the singular values are arranged in descending order: $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_n \geq 0$. For a given matrix $A$ we use the notation $\sigma_i(A)$ or $\lambda_i(A)$ to denote the $i^{th}$ (ordered) singular or eigen-value, respectively. If there is no danger of confusion, the explicit reference to the matrix will be suppressed. Recall that there is a useful relationship between the singular values of a matrix $A \in \mathbb{R}^{p \times q}$ and the eigenvalues of the related matrices $AA^T$ and $A^TA$:

$$\sigma_i(A) = \sqrt{\lambda_i(AA^T)} = \sqrt{\lambda_i(A^TA)}.$$  

(3)

where $i = 1 : \min(p,q)$. This connection will be used extensively in the analysis below.
C. Applying SVD to time series

In [5], the authors draw on SVD to address the following problems for time series:

1) Period extraction: Given a times series, \( x = (x_1, x_2, \ldots, x_n) \), reshape it as a \( p \times q \) matrix \( A \) (where \( p \) ranges between some judiciously chosen lower and upper value, and \( q = \text{floor}(n/p) \), is the nearest integer less than \( n/p \). The authors then introduce the singular value ratio

\[
SVR(p) = \frac{\sigma_1}{\sigma_2}
\]

(4)
to quantify the dominance of the first singular value over the second. High values of the SVR are then considered as an indicator of existence of strong underlying periodicities. Plotting \( SVR \) as a function of \( p \) allows one to spot peaks and identify underlying periodicities. It is not necessarily correct, however, and one must exercise caution when interpreting these graphs, as explained in Section II-B.

2) Data-driven times series approximation and decomposition: If in the expansion (2) all but the first \( r \) singular values are negligible, then truncating the expansion after \( r \) terms will still result in an excellent approximation of the full matrix \( A \) (and corresponding times series). Furthermore, the columns and rows that are retained, can often be interpreted as meaningful patterns (see Fig. 1). More precisely, for an arbitrary \( p \times q \) matrix \( A \) (using the notation established above) we know that the \((L_2) \) optimal approximation of rank \( p < r \) is given by:

\[
A_p = \sum_{k=1}^{p} \sigma_k U_k V_k^T
\]

and the Frobenius norm of the residual is given by

\[
||A - A_p||_F^2 = \sigma^2_{p+1}
\]
The gist of these observations is clearly illustrated in Fig. 1. The top panel shows a noisy block signal of length \( n = 1000 \) with a pronounced period \( p = 100 \) and \( q = 10 \) full cycles. In addition to the noise, there are three irregularly occurring spikes. After rewriting this time series as a \( 100 \times 10 \) matrix \( A \), we apply the SVD algorithm to obtain \( A = U S V^T \) where \( S \) is \( 100 \times 10 \) “rectangular diagonal” matrix with the 10 singular values on its main diagonal. The middle panel shows those ten singular values, clearly illustrating that all except the first two are negligible, which means that the matrix (and therefore the time series) can be accurately represented by truncating the expansion in (2) after the first two terms, i.e. rank-2 approximation (see Fig. 2).

Finally, the bottom panel of Fig. 1 displays the first three columns of \( U \) (left) and \( V \) (right), respectively. As they correspond to the most significant singular values, they are most important for the reconstruction of the signal. The \( U \)-columns cover one cycle and can be interpreted as successive profiles needed to reconstruct a generic cycle. In that sense, they are analogous to the various trigonometric basis functions in Fourier analysis. The \( V \)-columns, on the other hand, specify the amplitudes with which these basis functions need to be combined in order to reproduce the individual cycles observed in the data. Not surprisingly, the main profile \((U_1 \text{ top left})\) reflects the step-like behaviour seen during each cycle. As the amplitude of each of these steps is essentially constant, the 10 \( V_1 \)-entries displayed in the top-right panel show little variation. The \( U_2 \) profile (middle, left) captures the shape of the additional spikes that occur at irregular intervals. The positive values in the corresponding \( V_2 \)-coefficients (middle, right) clearly indicate in which intervals these spikes occur. Finally, the erratic appearance of both \( U_3 \) and \( V_3 \) are a further indication (in line with \( \sigma_3 \approx 0 \)) that all structural information has been extracted from the signal.

![Fig. 1. SVD application to pattern-extraction in noisy block signal. Top: Original data of noisy block signal with period 100. In addition to the noise there are three irregularly occurring spikes. Middle: The 10 singular values for SVR with period \( p = 100 \). Clearly, only the two first are significant and \( \sigma_1 \gg \sigma_2 \) confirming that \( p = 100 \) corresponds to a valid periodicity. Bottom: The first three columns of \( U \) (left) and \( V \) (right).](image-url)

Contribution of this paper and overview: The main contribution of this paper is to investigate more systematically the effects of noise (Section II-B) and signal levels (Section II-C) on the SVD spectrum of a time series with a known period. In Section III, we show how one can use this decomposition to detect and interpret outliers.
II. IMPACT OF SIGNAL- AND NOISE-LEVELS ON SINGULAR VALUES

As mentioned before, (4) was used to identify underlying periods in [5]. However, what was apparently not realized is that the singular values are influenced by relative and absolute levels of noise. Failing to recognize this interplay can result in biased or misleading results. For this reason, we will review and complement some earlier results.

A. Singular value spectrum of random matrices

In the introductory sections, we assumed that the matrix \( A \) was the superposition of some underlying periodic signal and independent noise. However, to disentangle the impact of signal and noise, we first focus on the effect of pure noise (i.e. random matrices). The spectral study of random matrices (i.e. matrices for which the entries are independent, identically distributed (i.i.d.) random variables) has been a very active research domain in recent years and uncovered a number of key insights (see e.g. [6], [7], [8]). One of the more striking results is the emergence of universality which basically says that as the size of the matrix grows, the distribution of the singular values becomes increasingly independent of the distribution of the individual entries. Put differently, as long as the mean and variance of the noise is kept constant, its actual distribution has very little influence on the distribution of the resulting singular values, assuming the size of the matrix is not too small. This surprising result is illustrated in Fig. 3 where we compare the singular values (averaged over 200 trials) of 50 × 50 random matrices for two different distributions of the individual matrix entries: standard normal and exponential (shifted to become zero-mean). The agreement of the singular values is striking.

In addition to the above result, we also know that rescaling the variance of the entries in a zero-mean random matrix induces a corresponding rescaling of the singular values:

\[
\sigma_i(\alpha A) = \alpha \sigma_i(A).
\]

This follows immediately from the observation that \( \alpha A = U(\alpha S)V^T \). In other words, the singular value ratio \( SVR = \sigma_1/\sigma_2 \) is not affected by a uniform increase in the noise variance. However, a shift in the mean of the noise does affect the SVR, as will be explained in the section below.

B. Impact of entries mean value

In the original papers [5], [9], it was not sufficiently appreciated how a shift in the mean value of the time series (the DC component) impacts on the SVR. This is important as failure to understand this issue introduces a major bias in the test values and could therefore result in erroneous conclusions. To address this issue, we compare the singular values of zero-mean \( p \times q \) random matrix \( A_0 \) and its mean-shifted version: \( \tilde{A} = A_0 + \alpha 1_{p \times q} \). Using the connection between singular values and eigenvalues expounded in (3), we can express any singular value \( \sigma(A) \) as:

\[
\sigma^2(A) = \lambda(AA^T) = \lambda(A_0A_0^T + \alpha 1_{p \times q}1_{p \times q}^T).
\]

Next, we make use of the standard results on Rayleigh quotients for eigenvalues which states that the dominant eigenvalue which basically says that as the size of the matrix grows, the distribution of the singular values.

\[
\sigma^2(A) \approx \lambda(A_0A_0^T + \alpha^2 1_{p \times q}1_{p \times q}^T).
\]

and so on for the successive eigenvalues.

Combining this with the approximation derived in (5), we get the following approximation for the first singular value of

\[
\lambda_1 = \max_{x \neq 0} \left\{ \frac{x^T M x}{x^T x} \right\} = \max_{|u| = 1} (u^T M u).
\]

Furthermore, if an unit vector \( u_1 \) realizes the above maximum, then the second largest eigenvalue is obtained as the solution of the constrained optimization problem:

\[
\lambda_2 = \max_{|u| = 1} (u^T M u) \quad s.t. \quad u_1 \perp u_1.
\]
A:

\[
\sigma^2(A) \approx \max_{|u|=1} u^T (A_0 A_0^T + \alpha^2 q 1_p 1_p^T) u = \max_{|u|=1} \left( u^T A_0 A_0^T u + \alpha^2 q u^T 1_p 1_p^T u \right) = \max_{|u|=1} \left( u^T A_0 A_0^T u + \alpha^2 q \left( \sum_i u_i \right)^2 \right) \tag{6}
\]

This derivation shows that

\[
\sigma^2(\lambda) \leq \max_{|u|=1} \left( u^T A_0 A_0^T u \right) + \alpha^2 pq = \sigma^2(A_0) + \alpha^2 pq, \tag{7}
\]

since from the Cauchy-Schwartz inequality it follows:

\[
\left( \sum_i u_i \right)^2 \leq \left( \sum_i u_i^2 \right) \left( \sum_i 1 \right) = p \quad \text{since } |u| = 1.
\]

However, in general the unit vector \( u \) that maximizes the Rayleigh quotient will not necessarily also maximize \( (\sum u_i)^2 \). In fact, for higher singular values, the number of orthogonal constraints on \( u \) increases proportionally, suggesting that on average \( \sum u_i \approx 0 \), and therefore \( \sigma^2(A) \approx \sigma^2(A_0) \). This is indeed exactly what is seen in numerical experiments (Fig. 4). Notice that the first singular value is very close to the maximal value obtained in (7) which is derived if optimizing both terms in (6), independently and simultaneously was had been done.

![Fig. 4. Comparison of the singular values of a matrix (10 × 10) with zero-mean entries (red) and shifted mean (α = 5). The dotted line indicates that (approximate) upper limit based on (7). Recall that the entries of the matrix \( A_0 \) are random numbers, but by shifting the global mean the underlying periodic signal is present.

Clearly, failing to remove the mean from a noisy time series would inflate the first singular value (and only the first one!) resulting in a upwardly biased value for the singular value ratio (SVR). This would reduce the power of an SVD-method in data mining applications such a blind screening. In the next section we will investigate what the impact of genuine underlying periodic signal is.

C. Impact of the underlying periodic signal

Suppose that we have a noisy but perfectly stationary and periodic time series \( x = (x_1, x_2, \ldots, x_n) \) with period \( p \). For the sake of simplicity, we assume that the data cover an integer number \( q = n/p \) of periods (cycles). As explained in Section I, we then use the first \( p \) observations to create a first column of the matrix \( A \), and the observations \( x_{p+1}, \ldots, x_{2p} \) to create the second column, and so on, until we end up with \( p \times q \) matrix \( A \). If the noise is very small, each column is essentially a copy of the first one and we can write:

\[
A \approx a_1 a_1^T
\]

where the \( p \times 1 \) column \( a \) represents the data for one period. In general, the data is noisy, however, and we model that by adding independent additive noise with variance \( \epsilon^2 \):

\[
A = a_1 a_1^T + \epsilon N.
\]

Here \( N \) is a \( p \times q \) matrix of independent, identically distributed (i.i.d.) noise variables with zero mean and unit variance.

To investigate the behaviour of the singular values we use the fact that

\[
\sigma^2(A) = \lambda(A^T A) = \lambda((a_1 a_1^T + \epsilon N)^T (a_1 a_1^T + \epsilon N)) = \lambda(a^2 a_1 a_1^T + \epsilon (N^T a_1 a_1^T + q \epsilon^2 (N^T N)))
\]

where \( a^2 = a^T a = |a|^2 \). Since the entries of the noise matrix \( N \) are independent, zero-mean and unit variance stochastic variables, we can make the following approximation for the \( q \times q \) matrix \( N^T N \):

\[
(N^T N)_{ij} = \sum_{k=1}^{q} N_{kj} N_{kj} \approx \begin{cases} q & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}
\]

The last approximation is obtained by taking the expected values and using the fact that \( E(N_{kj} N_{kj}) = 1 \) if \( i = j \), and zero otherwise. From this, we conclude that approximately:

\[
N^T N \approx q I_q
\]

Similarly, because the expectation value of the cross-term vanishes, using the linearity of the expectation operator yields:

\[
E((N^T a_1 a_1^T + q \epsilon^2 I_q) N) = E(N^T a_1 a_1^T) + q \epsilon^2 E(N) = 0.
\]

As a consequence, to a good approximation, the singular values of \( A \) can be identified as the eigenvalues of the following matrix:

\[
\sigma^2(A) \approx \lambda(a^2 a_1 a_1^T + q \epsilon^2 I_q).
\]

The structure of the matrix in the RHS allows us to arrive at some conclusions regarding the singular values. Since any vector is an eigenvector of the identity matrix, it suffices to focus on the first term which is a rank-1 matrix (as the product of a column and a row). This implies that all but one eigenvalue vanish, and since \( I_q \) is obviously an eigenvector of the form \( I_q a_1^T \) it follows that the maximal eigenvalue (and therefore, singular value) is approximately equal to

\[
\sigma_1(A) \approx q (a^2 + \epsilon^2)
\]

The subsequent singular values correspond to the eigenvectors which are mapped to zero by the rank-1 matrix and therefore are not influenced by the \( \epsilon^2 \) term:

\[
\sigma_i(A) \approx \sqrt{q} \epsilon \quad \text{(for } i \geq 2)\]
shift in the mean noise level. In this case, the mean
Section II-B where the first singular value was affected by a
realize that this observation is different from the result in
values grows proportional to
a
influenced by the signal
(signal). Notice how increasing the signal strength results in the corresponding
increments in the first singular value.

Put differently, these lower ranked singular values are not
influenced by the signal a, just by the noise. Notice also that
the difference between the first and the subsequent singular
values grows proportional to \( \sqrt{q} \), as it means that the more
cycles that are present in the data, the more pronounced the
difference. Furthermore, in many cases the noise-level \( \varepsilon^2 \) can
be neglected with respect to the strength of the signal (\( a^2 \)),
resulting in a further approximation:

\[
\sigma_1(A) \approx \sqrt{qa}.
\]

This is illustrated in Fig. 5 where we took a fixed noise-level
\( \varepsilon = 0.2 \) and a signal strength \( a \) which is a multiple of some
basic level \( a_0 = \sqrt{12.5} \) and \( a = ka_0 \) with \( k = 0, 1, 2, 3 \).
The number of full cycles in each case was equal to \( q = 10 \). We
therefore expect the first singular value for each of these signal
levels to be roughly equal to \( \sqrt{q} a_0 k \approx 11.2 k \). It is important
to realize that this observation is different from the result in
Section II-B where the first singular value was affected by a
shift in the mean noise level. In this case, the mean \( (1/p) \sum_i a_i \)
of the periodic signal a can still be zero, but it is its \( L_2 \) norm
(\( a^2 = |a|^2 \)) that is seen to affect the first singular value.

III. APPLICATION: DATA-DRIVEN OUTLIER IDENTIFICATION

In the preceding sections we have explored how the
singular value spectrum can be used to identify a low-rank
approximation of a time series and how to avoid misleading
biases in the process. These low rank approximations provide
us with a useful tool to identify and interpret outliers. As
an illustration, consider the data in the top panel of Fig. 6
which represents the hourly averaged power consumption of an
industrial cooler (installed in business offices) over roughly 6
months (January through early July, or \( n = 4368 \) data points).
This cooler works in tandem with two other coolers which
explains the burst-like character of the data. Since the activity
of this cooler is linked to human activity, it shows a clear
daily periodicity and we therefore performed an SVD with
\( p = 24 \) and \( q = n/p = 182 \). The plots in the next two rows
of Fig. 6 show (left) the first two \( U \)-columns (24 entries each)
and (right) the corresponding \( V \)-columns of length 182 each.

The two \( U \)-profiles are plausible: the first captures a
(weighted) average of the daily activity and therefore shows
some baseline-activity during the night which then ramps up
around 8am and returns to the baseline at about 8pm. The
additional contribution encoded in the second profile results in
a higher activity in the morning, but lower activity in the
afternoon.

The corresponding \( V \)-columns on the right specify the
appropriate coefficients with which these profiles should be
weighted to obtain the approximation (red graph in top panel of
Fig. 7). The \( V_1 \) values roughly mirror the raw data, but the
\( V_2 \) shows a spike that corresponds to the high value in
the 3rd burst, indicating that this high value is partly due to
an unusually high value in the morning. However, notice that
this spike is well modelled by the first two coefficients of the
SVD: as a consequence this high value does not result in a
corresponding high value for the residual (see bottom panel of
Fig. 7 and the zoomed-in version in Fig. 8). In fact, the third
burst shows a spike in the residuals but this corresponds to a
relatively low value, which however is not adequately captured
by a combination of the first two \( U \)-profiles.

So using this type of analysis we can easily make the
distinction between high values that are the result of unusual
but regular activity (encoded in \( U \)-profiles that correspond to
large singular values, and possibly lower values that however
cannot be adequately approximated by combining such prominent
data-driven profiles (i.e. "real" outliers).

IV. CONCLUSION

In this paper we have argued that the well-known singular
value decomposition (SVD) (which is usually applied to
matrix problems) can also be successfully applied to identify
periodic patterns (profiles) in time series. Furthermore, these
profiles are completely defined by the data and do not require
the specification of user-defined parameters, apart from the
period (which itself can be estimated using this approach). As
such, this methodology offers a purely data-driven approach
to adaptive signal approximation, and based on that, outlier
detection.

Moreover, we have shown that a judicious comparison
of the \( V \)-coefficients and residuals allows one to distinguish
between different ways in which data-points can be atypical
or salient. From a data mining perspective, this opens up
new ways of analyzing time series in a data-driven, bottom-
up fashion. However, it then becomes essential to thoroughly
understand how the spectrum of time series is influenced by
various characteristics of the signal and noise. In this paper,
we have extended the work in earlier papers by initiating a
more systematic analysis of these effects.

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Fig. 6. Top: Raw data: Hourly power consumption of cooler during first 6 months of the year. Bursts of activity are interspersed with periods of non-activity. Simple thresholding of the data would suggest that there are a number of unusually high values in the data, viz. in the 3rd, 5th and (possibly) 6th burst. Bottom two rows: First two U-profiles (left) and corresponding V-profiles obtained by SVD. For more details, see main text.
Fig. 7. **Top:** Rank-2 approximation (red) of the original signal (blue). **Bottom:** Corresponding residuals. Notice that the high peak in the third burst does not yield a high residual because it is adequately modelled by the extracted profiles.
Fig. 8. Detail of 3rd "burst" in data of Fig. 7. Top: Original (blue) and rank-2 approximation (red). Bottom: Residuals corresponding to top panel. Notice that the most prominent residual corresponds to a relatively low data peak, which however is unusual in shape.