SENSITIVITY OF PRINCIPAL COMPONENTS TO CHANGES IN THE PRESENCE OF NON-STATIONARITY

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ABSTRACT

Non-stationarity affects the sensitivity of change detection in correlated systems described by sets of measurable variables. We study this by projecting onto different principal components. Non-stationarity is modeled as multiple normal states that exist in the system even before a change occurs. The studied changes occur in mean values, standard deviations or correlations of the variables. Monte Carlo simulations are performed to test the sensitivity for change detection with and without knowledge about the non-stationarity for different system dimensions and numbers of normal states. A comparison clearly shows that the knowledge about the non-stationarity of the system greatly improves change detection sensitivity for all principal components. This improvement is largest for those components that already provide the greatest possibility for change detection in the stationary case.

Keywords  change detection · novelty detection · failure detection · non-stationarity · correlations · principal component analysis · eigenvalues · eigenvectors

1 Introduction

The detection of changes, novelty, failures or faults is a crucial task in numerous real world systems, such as industrial monitoring, energy generation, IT- and road-traffic, sensor networks, image processing and many more [1–4]. Early or even preemptive detection can help operations, avoid down-times and reduce costs in general. Techniques for such analysis can be roughly categorized into three groups: model-based methods, knowledge-based methods and data-driven methods [5]. While a lot of research is done in all directions, the first two groups require extensive knowledge about the monitored system and are therefore challenging and time-consuming. This has made the data-driven methods especially interesting for researchers in all fields [6].

Principal Component Analysis (PCA) [1,3,7] is one of those data-driven methods. It is commonly used as either a direct detection method or as a dimensionality reducing pre-processing. Here, data is projected into the space of the principal components, which are the eigenvectors of the covariance or correlation matrix for a system with multiple measured variables. Whether covariances or correlations are used depends on the system studied. The eigenvectors associated with the large eigenvalues are referred to as the major components. Without a change present, these carry most of the information on the behavior of the system. A projection onto the subspace of the major components includes the largest part of the variance of a data set. The other eigenvectors associated with small eigenvalues are referred to as minor components. For change detection one usually calibrates a normal parameter set of these projections. New data is then projected and compared to the normal space using, for example, Hotelling $T^2$-statistics or the sum of squared prediction error together with a threshold [8,9]. It has been applied to change detection in many different systems, including wind turbines [10], wastewater treatment plants [5], healthcare institutions [11] and traffic [12]. An important question is which of the principal components to look at. For the use-case of dimensionality reduction one generally

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employs a projection onto the major components [7]. However, the residual subspace, i.e. the minor components, is often most useful for outlier and change detection [1][13][14]. Shyu et. al. [15] proposed a method combining the components relating to the largest and the smallest eigenvalues for novelty detection. Recently, Tveten [16] studied the sensitivity of different principal components in a more structured and complete way confirming the high sensitivity of minor components to changes.

Many variants of PCA exist. They were developed to tackle different specific problems. Some better known ones include, but are not limited to, static and dynamic robust PCA [17][18], kernel PCA [19], dynamic kernel PCA [20], moving window PCA [21], recursive PCA [22] and incremental PCA [6]. The latter three tackle the important problem of non-stationarity. Many studied systems are subject to external influences or internal processes, that cause varying conditions. These lead to changes in the data, which do not represent novelty or failure. We refer the reader to the review [23] for an introduction to PCA on time-dependent data. A performance comparison is found in [24]. The problem of non-stationarity is also of on-going interest for other novelty detection methods [25][29][30].

Non-stationarity exists in different forms. First, a system can slowly evolve due to influences such as climate [27] or economic situation [31]. On the other side, external conditions can vary on shorter time-scales causing non-stationarity without an evolutionary trend [29][32][33]. Some systems also exhibit periodic non-stationarity [28]. A second distinction can be made in the type of non-stationarity: changes can occur in the absolute values of measured variables, their individual distribution or the relation between different variables. In simple terms these three categories represent novelty as changes in mean values, standard deviations or correlation structure respectively. Of course, this does not capture all possibilities. For example, distribution changes can also effect higher moments only. Furthermore, relations can be non-linear. However, this simplification already provided valuable insights in the sensitivity of principal components in stationary systems [16]. We study the importance of non-stationarity accordingly.

Of those three categories non-stationarity in the correlation structure is especially important for PCA (or any other method depending directly on the covariance or correlation matrix). The purpose of PCA is to find new coordinates that already incorporate the linear correlations in the system. If they change, i.e. the eigenvectors of the correlation matrix change their structure, the projections into PCA space are substantially different. Such a non-stationarity in the correlation matrix has been thoroughly investigated, for example, in financial markets [31][34], road traffic [32] and wind turbine data [33]. We assume that such a distinction into well-separated individual states is most likely to happen for a difference in correlation structure. At a certain point internal or external causes lead to a behavioral change. Changes in mean or standard deviation of variables might also exhibit such distinct states, but are more likely than a correlation structure to change continually. Therefore, our analysis will focus on correlation changes, but we will nevertheless study all types of change.

We aim with this study for a structured and comprehensive analysis of the sensitivity of principal components in the presence of non-stationarity, while trying to keep it simple enough that mechanisms can be easily understood. The non-stationarity is modeled as multiple possible normal states of the system. We study all three types of possible changes, but do not mix them. This means, if the change occurring at a certain point in time is of a certain type (mean value, standard deviation, correlation structure), the states will also differ in that same type. We base the study framework on the one used by Tveten [16] and extend it to incorporate non-stationarity. This facilitates comparison with the stationary case. We analyze the sensitivity of the principal components under the assumption that we know about the non-stationarity and compare it to the results obtained, if we did not know about the non-stationary behavior. Thereby, we can study how important knowledge about such a state-wise non-stationarity is for novelty detection with PCA.

We describe the idea of the experiment with a metaphor in section 2. In section 3 we introduce the problem and notations and set up the simulation framework in a general form. Section 4 contains the results of our simulation studies divided into subsections for the different change types. In these we also present the detailed simulation set up for each case. A summary of results and findings is found in section 5.

2 Analysis Concept

To facilitate easy understanding of the concept of our analysis before going into detail, we outline the simulation experiment with a simple example. Imagine a lamp with a light bulb that is burning with a certain color. Let us say it emits blue light. At a certain point in time \( t = \tau \) the light bulb changes its color slightly and we study from which viewing angle we can best detect this change. As a measure we take a color chart and estimate the difference \( h \) in points between the color before and after the change. Then we repeat this experiment time and again with different bulbs, different colors and different color changes while keeping track of the change detectability from each viewing angle. This is an easily imagined example for the stationary simulation experiment.
Now, let us assume that before \( t = \tau \) the light bulb burns with \( S \) different colors. At random intervals it changes its color, but all colors are equally likely over time. This represents non-stationarity in the way we are going to analyze. At time \( t = \tau \) a change occurs once again. However, the light bulb can be in any state \( s \in 1, \ldots, S \), i.e. burn with one of the possible colors. If we know of the non-stationarity and have a criterion to determine which color the lamp should have, we detect the change compared to the realized color \( s^* \). Once again we use our color scale and determine a point score \( h_1 \) from different viewing angles. However, we want to analyze how much improvement in the detectability of that change is caused by our knowledge about this non-stationarity. Therefore, we also calculate a detectability without it: We compare the color after the change occurs with the average color before the state. So, if our lamp would normally burn with either blue or red, we compare to a violet light. Again we take the color chart and note difference \( h_2 \) in points between changed color and average color before change from each angle.

To measure the increase in detectability with knowledge of the non-stationarity we have to compare the two measurements \( h_1 \) and \( h_2 \). The first one is easy enough, because it should produce the same results as the stationary case if our knowledge about the original state, i.e. color, of the light bulb is perfect. When measuring without knowledge about the non-stationarity we have to take into account that even without a change we will detect deviations from our assumed normal (the average state): At any given time the light will be red or blue, but we will compare it to violet and observe a difference \( h_{s, \text{norm}} \) between state \( s \) and the average state. This means that changes at \( t = \tau \) are detectable only if they differ stronger from the violet than our normal states (blue and red) do. We have to correct our measurement of difference by subtracting the maximum difference we measure without a change present: \( h_{2, \text{corr}} = h_2 - \max(h_{s, \text{norm}}) \). As in the stationary case we perform multiple Monte-Carlo simulations. The importance of knowledge about non-stationarity for change detection is then measured as \( h_1 - h_{2, \text{corr}} \).

3 Theory and Setup

In our analysis, the light bulb from the example above is a \( D \)-dimensional system with \( n \) observations \( x_t \in \mathbb{R}^D \) at times \( t = 1, \ldots, n \). We do not look at the time series themselves, but rather describe the system with mean values, standard deviations and Pearson-correlations. This description is complete only for Gaussian systems. We assume this to be the case for our study. At the time \( t = \tau \) a change occurs in the system, that can either influence mean, standard deviation or correlation structure of the observed variables. This is analogous to the change in color of the light bulb. For the stationary case the sensitivity to change in principal components was already analyzed by Tveten [16]. We extend it by the inclusion of non-stationarity. We assume that the system has \( S \) possible states and at every time is in one state \( s \in \{1, \ldots, S\} \) of them. For each of these states \( s \) we have a vector of means \( \mu^{(s)}_0 \), a vector of standard deviations \( \sigma^{(s)}_0 \) and a correlation matrix \( C^{(s)}_0 \). The index 0 indicates that these values refer to the system before the change at \( t = \tau \) occurs. In our example with the light bulb these three values together describe the color of the state. For further analysis, we standardize each state separately to mean zero and standard deviation one and denote standardization with a hat. This results in \( \hat{\mu}^{(s)}_0 = \mu^{(s)}_0 \) and \( \hat{\sigma}^{(s)}_0 = \sigma^{(s)}_0 \). Without knowledge about the \( S \) different states, two ways of measurement present themselves. One either measures just one set of parameters for the time span \( t = 1, \ldots, \tau \) as was assumed in [16] or one measures the parameters in epochs of a length \( \tau_{\text{ep}} < \tau \) and takes the averages. The second option offers the advantage that new data, in which one wants to test for change, is most likely also only available for a time span \( \tau_{\text{new}} < \tau \). The comparability of new and old data is therefore increased if epoch length and time span of the new data coincide, i.e. \( \tau_{\text{ep}} \approx \tau_{\text{new}} \). Correlations, for example, might be largely positive on a large time scale due to a global trend in values, but show more structure when measured on shorter time spans. Therefore we define the average state (analogous to the violet light of the light bulb example) as averages over epochs. Without loss of generality, we assume that each state \( s \) occurs for the same amount of time before the change and define the parameters of the average state as element-wise averages:

\[
\hat{\mu}_0 = \frac{1}{S} \sum_{s=1}^S \hat{\mu}^{(s)}_0, \tag{1}
\]

\[
\hat{\sigma}^2_0 = \frac{1}{S} \sum_{s=1}^S \hat{\sigma}^{(s)}_0, \tag{2}
\]

\[
\hat{C}_0 = \frac{1}{S} \sum_{s=1}^S C^{(s)}_0. \tag{3}
\]

We average the variance instead of the standard deviation. The average over the correlation matrix is also meant element-wise and is according to the centroid calculation in real data clustering in e.g. [31–34]. Standardization with the mean value and standard deviation of this average state will be denoted with a tilde: \( \tilde{\mu}_0 = \mu_0 \) and \( \tilde{\sigma}_0 = \sigma_0 \).
When the change happens at time $t = \tau$, it will affect the values we currently measure. In the light bulb example this would be the slight change of color. We denote these new values with an index 1 as $\mu_1, \sigma_1$ and $C_1$. Next, we need to decide how the data after the change should be standardized. In reality this question is, how the new (or possibly live) data of a system should be standardized before comparing it to the usual behavior. This is independent of whether or not non-stationarity has been accounted for. One can either standardize with the known pre-change values of the usual behavior or with the newly measured ones. If one measures only a single new data point, only the first option is feasible. Without loss of generality, we normalize with pre-change values. However, the correlation matrix after the change will not be a well-defined correlation matrix. Especially the entries on its diagonal will not be one. This does not present a problem for our analysis.

Including non-stationarity in the way of multiple pre-change states, we need to know what normal state the system would have been in after the change at $t = \tau$ to make the right comparison. We will denote this state with $s^*$. In reality this means that after having found multiple normal states, we need one criterion (or possibly several criteria) marking the states. For the current, theoretical analysis we assume that we simply know the state $s^*$ in the epoch after the change.

We can then standardize with the pre-change state parameters to get $\mu_1, \sigma_1$ and $C_1$. The hat denotes standardization with state parameters. To compare the sensitivity of principal components with knowledge of non-stationarity to the behavior or with the newly measured ones. If one measures only a single new data point, only the first option is feasible. In reality this question is, how the new (or possibly live) data of a system should be standardized before comparing it to the usual behavior. This is independent of whether or not non-stationarity has been accounted for. Hence, we will also calculate $\tilde{\mu}_1, \tilde{\sigma}_1$ and $\tilde{C}_1$, where the tilde denotes standardization with the average state parameters.

To analyze the sensitivity of principal components, we study the projections of the system onto the eigenvectors before and after the change. This is analogous to looking at the light bulb from different angles. Let $\{X_j, v_j\}_{j=1}^D$ be the normalized eigensystem of a state $s$ calculated from its correlation matrix $C_{s}^{(s)}$. Ordering is assumed from largest to smallest eigenvalue, i.e. $\lambda_1^{(s)} \geq \cdots \geq \lambda_D^{(s)}$. The projection of a data point $x_i$ onto the $j$-th component can then be calculated as $y_{j,t} = v_j^{(s)^T} x_i$. Furthermore, we want to compare projections onto these components for epochs rather than a single data point. If we know the vector of means $\mu$ and the correlation matrix $C$ of said epoch, we calculate the mean $\mu_j'$ and standard deviation $\sigma_j'$ of the projection onto the $j$-th eigencomponent by

$$
\mu_j' = v_j^{(s)^T} \mu \quad \text{and} \quad \sigma_j' = \sqrt{v_j^{(s)^T} C v_j^{(s)}}.
$$

We have dropped the state identification $(s)$ on the left side. This is possible, because projections are only ever needed into the average system and the system of $s^*$ so that no confusion with other states is possible. This allows us to keep the identifier, if it is actually the mean vector or the correlation matrix of the state, which is being projected. For example, the mean of projection onto component $j$ of the original state mean $\mu_j^{(s)}$ would read $\mu_j'^{(s)}$, whereas the projection of the changed state means $\mu_j$ would simply be $\mu_j'^{(s)}$. Then also the overline of an average state would translate into an overline on the projected notation. If standardization notation is necessary it will also translate. For comparison without knowledge about the non-stationarity also projections into the eigensystem $\{X_j, v_j\}_{j=1}^D$ of the average state are necessary. We denote these in the same way with a double prime:

$$
\mu_j'' = \overline{v_j^{(s)^T}} \mu \quad \text{and} \quad \sigma_j'' = \sqrt{\overline{v_j^{(s)^T} C v_j}},
$$

Having established the mean and standard deviation projections, we define the sensitivity as the Hellinger distance between the marginal distributions before and after the change. In the light bulb example this is the difference in points on the color chart. The squared Hellinger distance between two probability measures $P$ and $Q$ on the Lebesgue-measurable space $X$ with probability densities $p(x)$ and $q(x)$ is defined as

$$
H^2(P, Q) = \frac{1}{2} \int_X (\sqrt{p(x)} - \sqrt{q(x)})dx = 1 - \int_X \sqrt{p(x)q(x)}dx.
$$

It is easily calculated between two normal distributions $\mathcal{N}(\mu_1, \sigma_1^2)$ and $\mathcal{N}(\mu_2, \sigma_2^2)$ as

$$
H^2(\mu_1, \sigma_1, \mu_2, \sigma_2) = 1 - \frac{\sigma_1 \sigma_2}{\sigma_1^2 + \sigma_2^2} \exp \left\{ -\frac{1}{4} \frac{(\mu_1 - \mu_2)^2}{\sigma_1^2 + \sigma_2^2} \right\}.
$$

For this theoretical study it is more feasible than a data distribution comparison such as Hotelling $T^2$-statistics. For the Hellinger distance to be applicable - under the assumption of normal distributions - we do not need the actual
distributions. This allows us to simulate mean values, standard deviations and correlation matrices without having to generate the underlying data.

In Eq. (9) we have already adopted a notation that is easy to use for our application by writing the Hellinger distance as a function of the means and standard deviations of the normal distributions to compare. The projected $\mu$ and $\sigma$ are calculated as described above and fully describe the comparison. For example, the Hellinger distance between the pre-change projection of the state $s^*$ onto itself and the projection of the changed state into that same system with standardization with state pre-change parameters would read

$$H(\hat{\mu}_{j,0}', \hat{\sigma}_{j,0}', \hat{\mu}_{j,1}', \hat{\sigma}_{j,1}') = H_j(\hat{\mu}_{0}'(s^*), \hat{\sigma}_{0}'(s^*), \hat{\mu}_{1}', \hat{\sigma}_{1}')$$

(10)

For the right side we have simply taken the index $j$, which must always be equal for all arguments in $H$, and moved it from the arguments to the function for better readability.

We carry out different Monte Carlo simulations for changes in the correlation structure, the mean and the standard deviation. Each time we will assume that the other factors stay constant and the change type is the same for the occurring change at $t = \tau$ and in between the states. The detailed scheme for the simulation will always be given in the sections dealing with the results as these differ for the different change types. In general we will simulate normal states, calculate the average state and then simulate a change at $t = \tau$. We will always perform this for a multitude of normal states and for each of these for a multitude of change scenarios. The after-change data will be standardized and projected into the corresponding state eigensystem as well as the average eigensystem, Hellinger distances are calculated respectively. We then take the expectation value $\mathbb{E}_j$ over the Monte Carlo runs.

While in real data some fluctuations are always expected, which lead to non-zero Hellinger distances even without a change occurring, this is true for both the state and the average case and can therefore be neglected in a comparison. Remembering our light bulb example however, we have to correct the result without knowledge of the non-stationarity. In a non-stationary system with states there is an additional non-zero part of the Hellinger distance, if we do not know about the states. This is because the system would be in a state $s^*$, which is unequal to the average state even without change, but projected into the average eigensystem and compared to the average state. This would be additional noise in our change detection, that only occurs when not knowing about the non-stationarity. In our example this was the blue and red light already being different from the average violet color without a change. We therefore calculate the projections of the different states $s = 1, \ldots, S$ into the eigensystem of the average state. Of course, to do this, we need to standardize the state variables with the pre-change average parameters. We then calculate the Hellinger distances this would cause even without a change. The maximum of these distances is the threshold distance up to which we have to assume that the system behaves normally. We can only detect a real change at $t = \tau$ if it causes a Hellinger distance larger than the maximum one the states themselves cause. This maximum is subtracted from the Hellinger distance between the system with a change and the average state as only the difference between these two measures the detectability of a change in a non-stationary system without knowledge about this non-stationarity. As detectability can never be less than zero, we set negative values to zero. The subtraction is done inside the Monte Carlo runs. This ensures that the actual noise created by the state average comparison is taken as it can vary strongly depending on how different the original normal states are. We denote this corrected Hellinger distance with $\mathcal{H}_j$.

4 Results

The focus of our analysis lies in the difference between knowing and not knowing about the non-stationarity of the system. We present our results separately for the different types of change. This way it is easier to describe the simulation procedure including necessary standardization. We have tested our implementation to produce the same results as given by Tveten [16] for the stationary case, i.e. if we assume the number of states $S$ to be one. The results are shown in Fig. 1. The simulation procedures used for each different change type are described in the following sections.

We present the simulation and its results for correlation structure, mean value and standard deviation in Sec. 4.1, 4.2 and 4.3 respectively.

4.1 Change in correlation structure

We explore the sensitivity of principal components to a change in the correlation structure of the simulated variables. We think that this is the prominent use-case for PCA as changes in mean and standard deviation can also be detected by comparing their values directly. In contrast to the other scenarios, we do not have to worry about standardization issues as mean and standard deviation always stay the same. This is so, because we assume that the change does not influence these parameters and the normal states only differ in correlation structure. Hence, the vector of means $\mu_j^{(s)}$ and the
To compare states that emerged by applying changes to one random state, we simply change step 1. to the following:

1. Draw $S$ random correlation matrices $C_0^{(s)}$, $s = 1, \ldots, S$ of dimension $D$ using the method described in [36].

To obtain results for different combinations of dimension $D$, number of normal states $S$ and change sparsity $K$, we perform Monte Carlo simulations with various change scenarios. Thereby we get the estimate $\overline{H}_j$ as an average over all simulation runs. We simulate two scenarios, which differ in the method to create the different states $s$ that exist before the change. For one scenario they are random and unrelated to each other. For the second one we draw one random correlation matrix and obtain the other $S-1$ states by changing the first state in the same way that change is introduced at $t = \tau$ later on.

In the case of unrelated random states, our simulation follows the steps:

1. Draw $S$ random correlation matrices $C_0^{(s)}$, $s = 1, \ldots, S$ of dimension $D$ using the method described in [36].
2. Calculate the element-wise average correlation matrix $\overline{C}_0$ before the change.
3. Calculate the Hellinger distances $H_j(\overline{\mu}_0^n, \overline{\sigma}_0^n, \overline{\mu}_0^{n(s)}, \overline{\sigma}_0^{n(s)}), j = 1, \ldots, D$, $s = 1, \ldots, S$ between the states and the average state.
4. Draw a change sparsity $K$ uniformly from the set $\{2, \ldots, D\}$.
5. Draw a random subset $D \subseteq \{1, \ldots, D\}$ of size $K$.
6. Randomly draw the normal state $s^* \subseteq \{1, \ldots, S\}$ the system is in after the change at time $t = \tau$.
7. Draw a multiplicative change in correlation $a$ uniformly from the interval $\{0, 1\}$ and change $\rho_{i,d}$ to $a \rho_{i,d}$ for all $i \neq d \in D$, where $\rho_{i,d}$ denotes the off diagonal elements of $C_0^{(s^*)}$.
8. Calculate $H_j(\mu_0^{n(s^*)}, \sigma_0^{n(s^*)}, \mu_1^i, \sigma_1^i), j = 1, \ldots, D$ between changed state and state.
9. Calculate $H_j(\overline{\mu}_0^n, \overline{\sigma}_0^n, \mu_1^i, \sigma_1^i), j = 1, \ldots, D$ between changed state and average state.
10. Calculate the corrected Hellinger distance
    $$H_j(\overline{\mu}_0^n, \overline{\sigma}_0^n, \mu_1^i, \sigma_1^i) = \max_{s} (H_j(\mu_0^{n(s)}, \sigma_0^{n(s)}, \mu_1^i, \sigma_1^i)), j = 1, \ldots, D.$$
11. Repeat steps 4 to 10 for $10^3$ times.
12. Repeat steps 1 to 11 for $10^3$ times.

In step 7, we only apply decreases in correlation. We do this to avoid many indefinite changed matrices [16]. One can easily imagine that a multiplicative increase could often lead to correlation coefficients larger than one. If any indefinite matrices still occur, we use Higham’s algorithm [37] to find the closest positive-definite one. The results of such a simulation for $D = 20$ and $S = 3$ are seen in Fig. 2a. As mentioned before, correction of the Hellinger distance for the change detection with the average state is done inside the Monte Carlo runs. To obtain the single green line representing the correction values, we average over the Monte Carlo simulations.

To compare states that emerged by applying changes to one random state, we simply change step 1. to the following substeps and present the results in Fig. 2b.
We clearly see that in both scenarios the sensitivity is greatest for the minor components in the changed state to state distance. Another, more application oriented, reason is that many systems will not change or reverse their entire behavior, but remain the most sensitive. Knowledge about the non-stationarity enables a more sensitive change detection for different numbers of normal states and different dimensions. As expected, the increase in sensitivity is larger for more states. It is random and the other were obtained from it by applying changes.

a) Draw one random correlation matrix \( C_0^{(1)} \) of dimension \( D \) using the method described in [36].

b) Draw a change sparsity \( K \) uniformly from the set \( \{2, \ldots, D\} \).

c) Draw a random subset \( D \subseteq \{1, \ldots, D\} \) of size \( K \).

d) Draw a multiplicative change in correlation \( a \) uniformly from the interval \( \{0, 1\} \) and change \( \rho_{i,d} \) to \( a \rho_{i,d} \) for all \( i \neq d \in D \), where \( \rho_{i,d} \) denotes the off diagonal elements of \( C_0^{(1)} \).

e) Repeat steps b) to d) \( S - 1 \) times and use the changed correlation matrices as \( C_0^{(s)} \), \( s = 2, \ldots, S \).

We clearly see that in both scenarios the sensitivity is greatest for the minor components in the changed state to state comparison (red). This is, of course, in accordance with the non-stationary results (see Fig. 1) as we always compare to the correct normal state. The changed state to average state distance (blue) is larger than the one to the actual state for major components and a crossing point between the two appears towards minor components. This point lies with larger \( j \) for the case of related original states. However, as pointed out before, we need to correct this Hellinger distance by the maximum distance between the actual states and the average state (green). This corrected Hellinger distance is shown as the black line as long as it is larger than zero. It indicates the sensitivity of the change detection without knowledge about the non-stationarity. Its values are smaller than the ones with that knowledge for all principal components. In fact, they often lie below zero indicating no possible detection at all. The knowledge about non-stationarity greatly increases the possibility to detect changes.

For the case of unrelated states the blue and green line seem to be almost flat, indicating that all components possess the same sensitivity. This is an inherent feature of the averaging. If the correlation matrices of the states are all entirely random, the correlation structures tend to cancel each other out. Simply put, the off-diagonal elements of the average matrix tend towards zero. This results in meaningless eigenvector structures. This is further underlined by Fig. 3a showing the same results for \( S = 7 \). With more states the average matrix is closer to zeros on the off-diagonal and the blue and green line are even flatter. It is one of the reasons for the introduction of the scenario with related states. Another, more application oriented, reason is that many systems will not change or reverse their entire behavior, but rather change the behavior of certain groups of variables. In this case, we see in Fig. 3a that with an increased number of states the detection without knowledge about the non-stationarity becomes impossible, i.e. the corrected Hellinger distances is always smaller than zero. For \( S = 3 \) some detectability was given for minor principal components knowing just the average state, but this vanishes completely for \( S = 7 \).

In general, the increase in change detectability with knowledge about non-stationarity compared to without is measured by the difference between the changed state to state distance (red) and the corrected value for the average state (black). Results for this difference are shown in Fig. 4. With non-stationarity present in the analysis, the minor components remain the most sensitive. Knowledge about the non-stationarity enables a more sensitive change detection for different numbers of normal states and different dimensions. As expected, the increase in sensitivity is larger for more states. It

![PCA sensitivity with non-stationarity](image)
is also larger for unrelated normal states. Basically, these states are more different from each other than in the related case, so it is reasonable that the knowledge is more helpful here. We see, however, that for $S = 7$ for the largest $j$, where detectability is highest in general, the increase is larger for related normal states. As seen in Fig. 3 for $S = 7$ the corrected state to average state distance is always zero for both scenarios. So any difference in the sensitivity increase between the scenarios can only stem from a difference in the changed state to state distance. This is difference exists purely due to a technicality: Because correlation coefficients cannot be larger than 1 the changes applied here are multiplicative between 0 and 1, i.e. they only reduce correlation. As this is also true for the changes performed to obtain the related states, the related normal states have weaker correlations on average than in the scenario with random states. This leads to a change of the red curve in Fig. 2b and 3b. Here, the results are different from the stationary case, because the underlying set of matrices is changed. In general however, as long as different normal states exist, the knowledge about non-stationarity increases change detection sensitivity. As this is the main interest of the current study, we did not pursue this effect further, but it is interesting for future studies. Moving on, the difference in $D$ does not change the overall results. For small $j$ the increase is a bit larger for smaller dimensions, whereas a for large $j$ it is the other way around. With the sensitivity for change being greatest for the minor components, the knowledge about non-stationarity is very important also in high-dimensional systems. It is noteworthy that an increase in the dimension of the matrix to $D = 100$ means that the relative change sparsity can be much higher as the smallest value of changed dimensions remains at two independent of $D$. Our results are also valid for sparse changes.

In summary, the knowledge about state-wise non-stationarity is important for the detection of changes. The sensitivity increase with knowledge is largest for the minor components, where change detection without non-stationarity is already most sensitive. For the major components the increase is still detectable, but much smaller. We could speculate that PCA for dimension reduction in a system is therefore still quite possible without knowing about the non-stationarity, but this cannot be tested or verified in our setup and is not in the scope of this paper.

### 4.2 Change in mean

We now analyze the effect of changes in the mean values of variables. Again, we perform Monte Carlo simulations with various change scenarios to obtain results. The procedure in general is similar to the one used for changes in correlation, but the details change. We also simulate two different scenarios of normal states again: related and unrelated. In the case of unrelated, random states our simulation follows the steps:

1. Draw a random correlation matrix $C_0$ of dimension $D$ using the method described in [36], which is the same for all states.
2. Draw $S$ vectors of means $\mu_0^{(s)}$, where each element $(\mu_0^{(s)})_d$, $d = 1, \ldots, D$ is uniformly drawn from the interval $\{-3, 3\}$.

![Figure 3: Monte Carlo estimates for the Hellinger distances of projections onto the different eigenvectors in presence of a change in correlation structure. All results were calculated for $D = 20$ and $S = 7$. Values are only shown if they are larger than zero. In panel (a) all states were created randomly and unrelated to each other, whereas in panel (b) one state is random and the other were obtained from it by applying changes.](image-url)
3. Calculate the element-wise average vector of means $\overline{\mu}_0$ before the change.

4. Assume standardization with average pre-change parameters and calculate $H_j(\tilde{\mu}_0^\prime, \tilde{\sigma}_0^\prime, \mu_0^\prime(s), \sigma_0^\prime(s))$, $j = 1, \ldots, D$, $s = 1, \ldots, S$ between the states and the average state.

5. Draw a change sparsity $K$ uniformly from the set $\{2, \ldots, D\}$.

6. Draw a random subset $D \subseteq \{1, \ldots, D\}$ of size $K$.

7. Randomly draw the normal state $s^* \subseteq \{1, \ldots, S\}$ the system is in after the change at time $t = \tau$.

8. Draw an additive change in mean $\Delta \mu$ uniformly from the interval $\{-3, 3\}$ and set

\[
(\mu_1)_d = \begin{cases} 
(\mu_0(s^*))_d + \Delta \mu, & \text{if } d \in D \\
(\mu_0(s^*))_d, & \text{otherwise}
\end{cases}
\]

9. Assume standardization with known state pre-change parameters, i.e. $\hat{\mu}_0(s^*) = 0$ and

\[
(\hat{\mu}_1)_d = \begin{cases} 
\Delta \mu, & \text{if } d \in D \\
0, & \text{otherwise}
\end{cases}
\]

and calculate $H_j(\hat{\mu}_0^\prime(s^*), \hat{\sigma}_0^\prime(s^*), \hat{\mu}_1^\prime, \hat{\sigma}_1^\prime)$, $j = 1, \ldots, D$ between changed state and state.

10. Assume standardization with average pre-change parameters, i.e. $\tilde{\mu}_0 = 0$ and

\[
(\tilde{\mu}_1)_d = \begin{cases} 
(\mu_0(s^*))_d - (\overline{\mu}_0)_d + \Delta \mu, & \text{if } d \in D \\
(\mu_0(s^*))_d - (\overline{\mu}_0)_d, & \text{otherwise}
\end{cases}
\]

and calculate $H_j(\tilde{\mu}_0^\prime, \tilde{\sigma}_0^\prime, \hat{\mu}_1^\prime, \hat{\sigma}_1^\prime)$, $j = 1, \ldots, D$ between changed state and average state.

11. Calculate the corrected Hellinger distance

\[
H_j(\tilde{\mu}_0^\prime, \tilde{\sigma}_0^\prime, \hat{\mu}_1^\prime, \hat{\sigma}_1^\prime) = \max(H_j(\tilde{\mu}_0^\prime, \tilde{\sigma}_0^\prime, \hat{\mu}_1^\prime, \hat{\sigma}_1^\prime) - \max(H_j(\tilde{\mu}_0^\prime, \tilde{\sigma}_0^\prime, \hat{\mu}_0(s^*), \hat{\sigma}_0(s^*)), 0)), j = 1, \ldots, D.
\]

12. Repeat steps 5 to 11 for $10^5$ times.

13. Repeat steps 1 to 12 for $10^5$ times.

To have states that emerged by applying changes to one random state, we simply change step 2. to the substeps:

Figure 4: Sensitivity increase for a change in the correlation structure when knowledge about the state-wise non-stationarity is available compared to without that knowledge. Results are shown for different dimensions $D$ and for unrelated random states (simulation scenario 1) and related states, that were generated from one random state (simulation scenario 2). Panel (a) was simulated with $S = 3$ normal states, panel (b) with $S = 7$. 

States  
- related  
- unrelated

(a) $S = 3$  
(b) $S = 7$
PCA sensitivity with non-stationarity

Figure 5: Sensitivity increase for a change in mean when knowledge about the state-wise non-stationarity is available compared to without that knowledge. Results are shown for different dimensions $D$ and for unrelated random states (simulation scenario 1) and related states, that were generated from one random state (simulation scenario 2). Panel (a) was simulated with $S = 3$ normal states, panel (b) with $S = 7$.

1. Draw one vector of means $\mu_0^{(1)}$, where each element $(\mu_0^{(1)})_d$, $d = 1, \ldots, D$ is random from $\text{Unif}\{-3, 3\}$.
2. Draw a change sparsity $K$ uniformly from the set $\{2, \ldots, D\}$.
3. Draw a random subset $D \subseteq \{1, \ldots, D\}$ of size $K$.
4. Draw an additive change in mean $\Delta \mu \sim \text{Unif}\{-3, 3\}$ and set $$(\mu_s^{(1)})_d = \begin{cases} (\mu_0^{(1)})_d + \Delta \mu, & \text{if } d \in D \\ (\mu_0^{(1)})_d, & \text{otherwise}, \ s \neq 1 \end{cases}$$
5. Repeat steps b) to d) $S - 1$ times and use the changed vectors of means as $\mu_s^{(s)}$, $s = 2, \ldots, S$.

As we saw in section 4.1, the most interesting result is the increase in sensitivity with knowledge about the non-stationarity compared to change detection without said knowledge. These simulation results are shown in Fig. 5. We see a clear increase in sensitivity for all simulated parameters. As before with changes in correlation structure, the knowledge about non-stationarity is slightly more important when the original normal states are related to each other and therefore not entirely different for $S = 3$. For $S = 7$ this difference is no longer visible. This is because the corrected Hellinger distances are always zero here and the changed state to state distances are not substantially different between the two scenarios. There is no influential change in the underlying set of states in contrast to the one seen in Sec. 4.1.

We again conclude that the non-stationarity is in general important for change detection. The increase seems to be more important for small $j$, i.e. major components, as compared to the results in section 4.1. However, this is most likely due to the fact that the change sensitivity without non-stationarity already exhibits the same changes in their dependency on $j$ (see Fig. 1).

4.3 Change in standard deviation

Finally, we analyze the sensitivity for changes in standard deviation in the presence of non-stationarity. The basic Monte Carlo process is the same, but once more the details are different. We simulate related and unrelated normal states again. In the case of unrelated, random states our simulation follows the steps:

1. Draw a random correlation matrix $C_0$ of dimension $D$ using the method described in [36], which is the same for all states.
2. Draw $S$ vectors of standard deviations $\sigma_0^{(s)}$, where each element $(\sigma_0^{(s)})_d$, $d = 1, \ldots, D$ is uniformly chosen from the interval $\{\frac{1}{3}, 2\}$. 
3. Calculate the element-wise average vector of variances $\sigma_0^2$ before the change. Then take the square root to get the average standard deviations.

4. Assume standardization with average pre-change parameters. Then $\tilde{C}_0$ is a well-defined correlation matrix with ones on its diagonal. $\tilde{C}_0^{(s)}$ is calculated from the state covariance matrix $\Sigma_0^{(s)} = \text{diag}\left(\sigma_0^{(s)}\right) \tilde{C}_0^{(s)} \text{diag}\left(\sigma_0^{(s)}\right)$ as follows: $\tilde{C}_0^{(s)} = (\text{diag}\left(\sigma_0\right))^{-1} \Sigma_0^{(s)} (\text{diag}\left(\sigma_0\right))^{-1} \tilde{C}_0^{(s)}$ is not a well-defined correlation matrix. We then calculate the Hellinger distance $H_j(\tilde{\rho}_0^{(s)}, \tilde{\sigma}_0^{(s)}, \tilde{\mu}_0^{(s)}, \tilde{\sigma}_0^{(s)})$, $j = 1, \ldots, D$, $s = 1, \ldots, S$ between the states and the average state.

5. Draw a change sparsity $K$ uniformly from the set $\{2, \ldots, D\}$.

6. Draw a random subset $D \subseteq \{1, \ldots, D\}$ of size $K$.

7. Randomly draw the normal state $s^* \subseteq \{1, \ldots, S\}$ the system is in after the change at time $t = \kappa$.

8. Draw a multiplicative change in standard deviation $\Delta \sigma$ uniformly from either the interval $[\frac{1}{3}, 1]$ (decrease) or the interval $[1, 3]$ (increase) with the same probability for the two options. Set

$$\sigma_1 = \begin{cases} \left(\sigma_0^{(s^*)}\right)_d \cdot \Delta \sigma, & \text{if } d \in D \\ \left(\sigma_0^{(s^*)}\right)_d, & \text{otherwise} \end{cases}$$

9. Assume standardization with known state pre-change parameters. Then $\tilde{C}_0^{(s^*)}$ is a well-defined correlation matrix with ones on its diagonal and $\tilde{C}_1$ is calculated analogous to the description in step 4. Then calculate the Hellinger distance $H_j(\tilde{\rho}_0^{(s^*)}, \tilde{\sigma}_0^{(s^*)}, \tilde{\mu}_0^{(s^*)}, \tilde{\sigma}_0^{(s^*)})$, $j = 1, \ldots, D$ between changed state and state.

10. Assume standardization with average pre-change parameters. Then $\tilde{C}_0$ is a well defined correlation matrix and $\tilde{C}_1$ can be calculated analogous to the procedure in step 4. Then calculate the Hellinger distance $H_j(\tilde{\rho}_0^{(s)}, \tilde{\sigma}_0^{(s)}, \tilde{\mu}_0^{(s)}, \tilde{\sigma}_0^{(s)})$, $j = 1, \ldots, D$ between changed state and average state.

11. Calculate the corrected Hellinger distance $H_j(\tilde{\rho}_0^{(s)}, \tilde{\sigma}_0^{(s)}, \tilde{\mu}_0^{(s)}, \tilde{\sigma}_0^{(s)}) = \max(H_j(\tilde{\rho}_0^{(s)}, \tilde{\sigma}_0^{(s)}, \tilde{\mu}_0^{(s)}, \tilde{\sigma}_0^{(s)}), 0)$, $j = 1, \ldots, D$.

12. Repeat steps 5 to 11 for $10^3$ times.

13. Repeat steps 1 to 12 for $10^3$ times.

To have states that emerged by applying changes to one random state, we simply change step 2. to the substeps:

a) Draw one vector of standard deviations $\sigma_0^{(1)}$, where each element $\left(\sigma_0^{(1)}(d)\right)_d$, $d = 1, \ldots, D$ is random from $\text{Unif}\{\frac{1}{3}, 2\}$.

b) Draw a change sparsity $K$ uniformly from the set $\{2, \ldots, D\}$.

c) Draw a random subset $D \subseteq \{1, \ldots, D\}$ of size $K$.

d) Draw a multiplicative change in standard deviation $\Delta \sigma$ uniformly from either the interval $[\frac{1}{3}, 1]$ (decrease) or the interval $[1, 3]$ (increase) with the same probability for the two options. Set

$$\sigma_0^{(s)} = \begin{cases} \left(\sigma_0^{(1)}\right)_d \cdot \Delta \sigma, & \text{if } d \in D \\ \left(\sigma_0^{(1)}\right)_d, & \text{otherwise} \end{cases}$$

$\sigma_0^{(s)}$, $s = 2, \ldots, S$.

e) Repeat steps b) to d) $S - 1$ times and use the changed vectors of standard deviations as $\sigma_0^{(s)}$, $s = 2, \ldots, S$.

The results for detection sensitivity increase due to knowledge about the non-stationarity are shown in Fig. [3]. It seems to be small for a large number of components $j$, especially the major components. As was the case with a comparison between changes in mean and correlation structure, this is largely due to the different sensitivity in the stationary case (see Fig. [1]). The curve of the increase always shows a similar behavior over $j$ as the stationary sensitivity itself shows. This underlines the importance of knowledge about non-stationarity as one would use these components for practical applications.

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1. We discussed in section 3 that simply taking the average is probably closest to a real use case. In the case of non-changing means between the states and with every state appearing for the same amount of time, this actually gives the correct variance over all states.
Figure 6: Sensitivity increase for a change in standard deviation when knowledge about the state-wise non-stationarity is available compared to without that knowledge. Results are shown for different dimensions $D$ and for unrelated random states (simulation scenario 1) and related states, that were generated from one random state (simulation scenario 2). Panel (a) was simulated with $S = 3$ normal states, panel (b) with $S = 7$.

5 Conclusion

We studied the sensitivity for change detection of principal components in non-stationary, correlated systems with multiple time series measurements. The non-stationarity was defined as the possibility for the system to be in multiple, distinctly different normal states prior to the change. Our study was based on the one conducted by Tveten [16] for stationary time series. Accordingly, the changes, which should be detected, were either to correlation structure, mean values or standard deviations of the time series. For simplicity, we constricted the study to those scenarios, where the normal states differ in the same property, in which the change also occurred. We analyzed how the detectability of the change varied for each principal component depending on the knowledge of the non-stationarity.

We found that in general the knowledge about the non-stationarity always increases the sensitivity for change detection. The increase is dependent on the principal component on which the data was projected. This dependency is quite similar to the one that was already found for the pure sensitivity for change detection in a stationary system. This means that where sensitivity for change is highest, also the increase gained by knowledge about the non-stationarity is highest. Usually this is for the minor components, i.e. the eigenvectors associated with small eigenvalues. This is reasonable as they represent behavior that is entirely unusual for a system in its normal state. When a change occurs, it can be seen very easily in those projections. If they are mixed up due to multiple normal states, this clear possibility to see changes is diminished. This underlines the importance of non-stationarity for direct uses of PCA for change detection. Usage of PCA for dimensionality reduction by keeping only projections on major components will probably be less influenced by this. This is an interesting aspect to study in the future. Other methods depending on eigenvectors for change detection (e.g. Mahalanobis distance) were not directly studied, but we think it likely that their sensitivity to change could also be increased by the consideration of multiple normal states. Our results are true for all three different types of changes and states. We further analyzed two scenarios: Unrelated and related normal states. We found that the sensitivity increase is usually greater for unrelated states, which is reasonable as the non-stationarity has a stronger effect in this case. We want to point out once again, that the use of multiple normal states for change detection in real applications is only possible, if a criterion can be found to identify which normal states new data should be compared to. The purpose of the present study was to develop the concepts and to provide the necessary tools. In a forthcoming study, we will analyze empirical correlation matrices for wind farm data. As this requires several rather specific intermediate steps, we find it useful to present this analysis separately from the conceptual aspects.
Our results clearly show that non-stationarity should be taken into account if one undertakes change, novelty or failure detection using principle component analysis.

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