A principle feature analysis

Tim Breitenbach* Lauritz Rasbach† Chunguang Liang‡ Patrick Jahnke§

Abstract

A key task of data science is to identify relevant features linked to certain output variables that are supposed to be modeled or predicted. To obtain a small but meaningful model, it is important to find stochastically independent variables capturing all the information necessary to model or predict the output variables sufficiently. Therefore, we introduce in this work a framework to detect linear and non-linear dependencies between different features. As we will show, features that are actually functions of other features do not represent further information. Consequently, a model reduction neglecting such features conserves the relevant information, reduces noise and thus improves the quality of the model. Furthermore, a smaller model makes it easier to adopt a model of a given system. In addition, the approach structures dependencies within all the considered features. This provides advantages for classical modeling starting from regression ranging to differential equations and for machine learning.

To show the generality and applicability of the presented framework 2154 features of a data center are measured and a model for classification for faulty and non-faulty states of the data center is set up. This number of features is automatically reduced by the framework to 161 features. The prediction accuracy for the reduced model even improves compared to the model trained on the total number of features. A second example is the analysis of a gene expression data set where from 9513 genes 9 genes are extracted from whose expression levels two cell clusters of macrophages can be distinguished.

1 Introduction

Data driven modeling and data driven decision making are rational ways of exploiting information contained in data to turn it into knowledge. The knowledge obtained from a set of data in turn may help to understand processes better from which the data is measured. The better understanding of the dynamics in a system may be used to steer or influence the observed process such that we obtain our desired output. However, the more accurate our demands become concerning the difference between the predicted and the real outcome of a process or experiment, respectively, the more variables need to be measured. Depending on this accuracy requirement, measuring variables that describe small effects on the outcome cannot be neglected. A growing amount of data is challenging with respect to storage and processing capabilities. Furthermore, the analysis of the data needs more effort to obtain the desired insights into the system’s relations due to the growing degrees of freedom. The research field of molecular biology illustrates this development. In the beginning, the nineteenth century, only light microscopes were available to observe cells, e.g. via staining. Nowadays there are technologies available like single cell RNA sequencing [44, 41, 42] allowing to measure the gene expression levels of a bulk of cells resolved at a level of an individual cell. This allows for modeling the inner mechanisms of cells very detailed once we are able to see the relations in the amount of data. Due to the amount of data it is very purposeful to use computational methods for the analysis of the data [5].

The aim of this work is to provide a framework including an algorithmic pipeline for the task of finding the relevant features for modeling and prediction by identifying features that are functions of other features. Furthermore, the relations in the considered data set are systematically analyzed by structuring the dependencies within all the data set’s features and quantities. From this analysis the building of reasonable and purposeful models of the underlying processes may start.

The key issue with data sets is that not all measured features are independent of each other. Consequently, measuring more features may not increase the amount of information contained in the data set with respect to

*Biozentrum, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany; tim.breitenbach@mathematik.uni-wuerzburg.de
†Department of Computer Science Distributed Systems Programming, Technische Universität Darmstadt, Hochschulstraße 10, 64289 Darmstadt, Germany; rasbachlauritz@googlemail.com
‡Biozentrum, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany; liang@biozentrum.uni-wuerzburg.de
§Department of Computer Science Distributed Systems Programming, Technische Universität Darmstadt, Hochschulstraße 10, 64289 Darmstadt, Germany; jahnke@dsp.tu-darmstadt.de
the modeling or prediction task while increasing only the size of the data set. The information which features are mutually independent is a valuable insight for several reasons. On the one hand, we can build a mechanistic model starting with independent features as input variables and step by step model other features as functions of them. For example, models can be built with differential equations or by fitting functions with regression. On the other hand, taking only the variables with the significant information helps to reduce the curse of dimensionality. Consequently, the degrees of freedom are reduced and e.g. a neuronal network is trained with the compressed information. Concentrating the information ensures that the prediction power of each selected feature clearly sticks out through the noise of the data set. Thus the concentration improves the signal-to-noise-ratio and the prediction accuracy compared to case where no selection of the features takes place. The presented framework results in smaller models that still carry the relevant information. In particular, the size of neuronal networks is reduced which may simplify their analysis concerning explainable AI [36]. Moreover, there are many methods [35, 40, 38, 9, 23, 25] providing explanations of the output of black-box machine learning models. A machine learning model with an as small number of independent input variables as possible will enhance their performance as well with respect to computational issues and providing an easy but meaningful explanation.

In the following, we list the main advantages of our framework.

- Applicable for linear and non-linear relations between the features
- Model reduction based on the original features without loss of information preserving prediction quality
- Increasing performance due to focussing on the relevant features
- Structures data sets and relations between features

The advantages listed above are achieved by the combination of a statistical test of independence for two features and a minimal cut algorithm from graph theory which clearly identifies structures being typical for features that are functions of other features. The presented framework consists of the combination of the following two building blocks. A chi-square test [15] testing for independence of two features and the minimal cut decomposition from graph theory [13]. The information about the independence of two features is modeled into an undirected graph, called dependency graph, where the nodes represent the features. There is an edge between two nodes if the corresponding features are not independent of each other. More specific, the values taken by each feature are not independent of each other. The second building block is a minimal cut algorithm that dissects that graph iteratively into disjunct subgraphs meaning that the removed nodes correspond to features that are not independent of the left mutually independent subgraphs. Moreover, given the values of the corresponding features of such a subgraph we cannot infer the values of the features of the other subgraphs. However, given the values of the features corresponding to all the disjunct subgraphs, we may infer the vales of the removed features. Iteratively we construct a set of independent features. The presented framework does not exclusively require the chi-square test. Any test that measures the dependency between two random variables can be used to generate such a graph defined above. The key point is to use a minimal cut algorithm to dissect the corresponding graph since this procedure identifies typical structures that features form when they are a function of other (stochastically independent) features. In this context features are also called variables or arguments of a function.

Once we have this set of independent features of which the other features are not independent, we can further process this set by choosing only variables of which output variables are not independent. These output variables are the values that we would like to calculate given a set of input variables. The connection between these input variables and the output variables, i.e. the model that connects these variables, can be generated with several methods. These can be machine learning models like neuronal networks, support vector machines or decision trees that learn the relations of this independent variables to the output variables. Furthermore, we can analyze these dependencies by fitting functions by regression models, for example to get a deep understanding of how the variables are connected. Another kind of mechanistic modeling is with partial or ordinary differential equations. With these type of equations we model the variation of the output variables depending on the input variables with respect to space or time.

An application of ordinary differential equations where we have many possible input variables and need to find out the relevant input variables to start from is the modeling of gene regulatory networks like in [10] [19]. In these networks, the regulation of genes by the expression level of other genes is modeled. In this field, our framework can help to identify the topology of the network that models which gene activates or inhibits the expression of other genes. The variables in the scenario of gene regulatory networks represent the expression levels of the corresponding genes, the transcription levels of RNA or translation levels of proteins. We can identify the basic genes or proteins from where we can start to generate the network.
In Section 2, we introduce the framework of our principle feature analysis (PFA) and discuss the corresponding algorithms.

In Section 3, we apply the framework to filter out the relevant features, called metrics, of a data center environment to classify if a current measurement of the metrics implicates that the corresponding data server is in an error state or if the data server is in a normal working status. Furthermore, the presented method is evaluated by comparing it to other related methods among other things.

A further field of application of the presented framework is in bioinformatics. In particular, the analysis of gene expression data to find out the significantly expressed genes corresponding to different cell states. For example, if one labels cells with pathological and physiological according to the cell’s state, the analysis with the presented framework may provide the genes that are responsible for making the difference in the behavior of a cell to be physiological or pathological. By the PFA one may identify the signal cascades causing genes or proteins which are relevant in a tumor setting for example. We demonstrate the extraction of relevant genes to differ two cell clusters of macrophages in Section 4.

In Section 5, we relate the PFA to existing methods. A Discussion about the chi-square test and a Conclusion complete this work.

In the Appendix, we give technical details about dealing with features with a continuous co-domain and discuss requirements to apply the chi-square test for our framework.

2 The principle feature analysis (PFA)

In this section, we describe the principle feature analysis. The description includes all the necessary definitions, algorithms, examples to illustrate the analysis and a theoretical result. We start with describing the basic idea and subsequent we explain the framework in detail.

The idea in a nutshell: our first step for analyzing the relation between the features is to test if two features are stochastically independent. If the features are stochastically independent, the value of one feature does not influence the value of the other feature. On the other hand, features that are a function of other features are not independent of these input features. The key issue is to identify such structures that functions form with their input variables. Thus we distinguish between features that are functions and features that are the input variables or arguments of functions. The independency is evaluated based on the result of a suitable statistical test with which we test the hypothesis that two features are stochastically independent. The suitable stochastic test has to provide a probability for the test’s result of the investigated instance of values of the corresponding features given the hypothesis is true. Since with a measurement we can only pick a specific instance of a random experiment, we have to define a measure on which we decide to reject the hypothesis. For this purpose, we have to define a threshold, we call it the level of significance. If the probability of the test is below this threshold, we consider it too unlikely that the hypothesis holds in the considered tested instance and we rather assume that the opposite of the hypothesis is correct, i.e. the features are stochastically not independent. From the information about the independency of each two features, we generate a graph where each node represents a feature. The binary result of the test of independency is encoded with unweighted and undirected edges. An edge between two nodes indicates that the corresponding features are statistically not independent based on our predefined level of significance. If two features are stochastically independent, then these two features do not influence each other. Consequently, there is no functional relation between such features with which we could calculate the value of one of these features given the value of the other one in a measurement. In contrast, features which are a function of other features do stochastically depend on them since the outcome of the function is influenced by the values of the input features. The nodes of independent features can be connected via paths over nodes of features that are a function of these mutually independent features. The crucial observation is now that features that are functions of other features are linkers of disconnected nodes or subgraphs, respectively. Removing such linker nodes from the graph may correspond to identifying features that are functions of other features. As we see later, any method that finds a set of nodes of minimal cardinality such that the remaining graph consists of at least two disjunct subgraphs is suitable for identifying the linker nodes. Moreover, the minimality of the set will ensure that no independent feature is removed. We repeat dissecting the graph by removing sets of minimal cardinality until only complete subgraphs are left, i.e. subgraphs in which each node is connected by an edge with any other node of this subgraph. The features of these resulting subgraphs are considered as the input features from where the modeling can start and construct the dependencies to interesting features that correspond to nodes that have been removed. In addition, from the input features we can identify these features on which a considered quantity, which is supposed to be modeled, depends with a further suitable statistical test before we start the modeling. In Figure 1, we summarize the workflow and give sites in this section where the topic is investigated.
Choose a test for independence of two features:
Paragraph after (1), Remark 8

Choose a threshold on which to decide for independence:
After (2)

Generate the corresponding graph:
Paragraph after (2)

Choose a strategy to dissect the graph:
Algorithm 1

Dissect the graph until only complete subgraphs are left:
Algorithm 1, Lemma 1, paragraph after Remark 6, Example 7

Analyze complete subgraphs:
Discussion after Example 2 and before Example 3

Choose features corresponding to nodes of complete subgraphs to model quantities with:
Paragraph before Example 3, Remark 4, Example 9

Figure 1: Workflow of Section 2 with sites in the text where to find information about the topic.

In the following, we describe the framework in detail. Let a set of \( n \in \mathbb{N} \) random variables be denoted with \( \hat{X} = \{x_1, ..., x_n\} \) where each random variable is denoted with \( x_i : \Omega \to \mathbb{R}, \omega \mapsto x_i(\omega) \) for all \( i \in \{1, ..., n\} \) with \( \Omega \) a measurable space. We refer to [20, Chapter 1] for basic definitions of the topic of stochastics. Furthermore, let \( Y = \{y_1, ..., y_m\}, m \in \mathbb{N} \) be a set of output random variables where it holds \( y_j : \Omega \to \mathbb{R}, \omega \mapsto y_j(\omega) \) for all \( j \in \{1, ..., m\} \). In this framework, each considered feature is modeled with a random variable in the sense that the value that a feature takes is a measurement of an outcome of a random experiment. In the following the features will be denoted with random variables.

The subset of \( \hat{X} \) of all principle variables, i.e. the variables corresponding to the nodes of the resulting complete subgraphs, is denoted with \( X' \subseteq \hat{X} \). The subset of \( X' \) of which variables in \( Y \) are not independent is denoted with \( X \subseteq X' \).

We recall the concept of stochastically independent random variables, see also [20, Chapter 2], since this is an essential ingredient of the presented work. We remark that the framework is not limited to the concept of stochastic independence. Any measure that describes the relation between two variables to define what the values of one variable tells about the value of the other one can be used. Let us consider two random variables \( A : \Omega \to Z_A, \omega \mapsto A(\omega) \) and \( B : \Omega \to Z_B, \omega \mapsto B(\omega) \) where \( Z_A \) is a set of \( k \in \mathbb{N} \) elements that \( A \) can take and \( Z_B \) is a set of \( l \in \mathbb{N} \) elements that \( B \) can take. The elements of \( Z_A \) and \( Z_B \) are called events. We say that two variables are stochastically independent if the equation

\[
P \left( A = z_A^i \text{ and } B = z_B^j \right) = P \left( A = z_A^i \right) P \left( B = z_B^j \right)
\]

is fulfilled with \( z_A^i \in Z_A, z_B^j \in Z_B \) for all \( i \in \{1, ..., k\} \) and \( j \in \{1, ..., l\} \) where \( P \) is the function that gives the probability for the random variables taking the corresponding event as denoted with the argument of \( P \) in the brackets. The function \( P \) is called the probability function. We remark that if the set of variables \( \hat{X} \) contains variables with a continuous co-domain, i.e. the range of values a variable can take, the co-domain of such a variable needs to be discretized for applying (1). A possible implementation is shown in the appendix, see Algorithm 4.

In the following, we discuss the test of independence of two random variables from \( \hat{X} \). For this purpose, it is tested if these random variables fulfill (1). Due to the finiteness of the number of measurements and the possibly non-deterministic dynamics of a system, we cannot expect that our measured distribution of our random variables exactly matches its real distribution according to which each random variable distributes its outcomes. Consequently, both sides of (1) will not exactly be equal even in the case where the real distribution of the random
variables, which we actually mostly do not know, fulfill (1) perfectly. However, we can test if the equality holds on a level of significance which means that it can be tested how likely it is to obtain such different values of the left and right hand side of (1) given that both random variables are independent. In this work, a chi-square test as follows. Both sides of (1) can be each considered as a discrete probability distribution function with regard to the domain \( i \in \{1, \ldots, k\} \) and \( j \in \{1, \ldots, l\} \). Before we go ahead, we write (1) into an equivalent form where the frequencies of the events are considered. We multiply (1) by the total number of measurements \( N \) for all \( i \in \{1, \ldots, k\} \) and \( j \in \{1, \ldots, l\} \). Then the observed frequency for the event \( A = z_A^i \) and \( B = z_B^j \) is given by

\[
f_O : \{1, \ldots, k\} \times \{1, \ldots, l\} \to \mathbb{R}, (i,j) \mapsto f_O(i,j) = P(A = z_A^i \text{ and } B = z_B^j) \cdot N
\]

and the expected frequency of this event is given by

\[
f_E : \{1, \ldots, k\} \times \{1, \ldots, l\} \to \mathbb{R}, (i,j) \mapsto f_E(i,j) = P(A = z_A^i) P(B = z_B^j) \cdot N
\]

assuming that the \( A \) and \( B \) are independent, meaning the outcome of one random variable does not influence the outcome of the other one. Since (1) has to hold for all \( i \in \{1, \ldots, k\} \) and \( j \in \{1, \ldots, l\} \), we equivalently test if both distributions with the corresponding frequencies of the events are the same. For this purpose, the measure

\[
\chi^2 := \sum_{i=1}^{k} \sum_{j=1}^{l} \frac{(f_O(i,j) - f_E(i,j))^2}{f_E(i,j)} \tag{2}
\]

is used to test, if the observed distribution of the frequency \( f_O \) equals the expected distribution of the frequency \( f_E \) assuming the independence of the two random variables \( A \) and \( B \). If both variables are stochastically independent and thus both sides of (1) are supposed to be equal, the measure \( \chi^2 \) is supposed to be small. Due to the finite number of measurements and the non-deterministic dynamic of the random variables, it may probably happen, that the outcome of our measurement process is such that, although the random variables are independent and thus (1) holds for the real distributions, the measure \( \chi^2 \) is greater than zero. In this case, we need to decide on a predefined level of significance \( \alpha > 0 \) if we consider \( A \) and \( B \) as independent random variables though. In the case of independent random variables, \( \chi^2 > 0 \) is considered as a result of random fluctuations. If we define

\[
\chi_{ij} := \frac{f_O(i,j) - f_E(i,j)}{\sqrt{f_E(i,j)}}, \tag{3}
\]

for any \( i \in \{1, \ldots, k\} \) and \( j \in \{1, \ldots, l\} \), then \( \chi^2 \) is chi-square distributed if each \( \chi_{ij} \) is normally distributed with the expectation zero and the variance one and mutually independent for all \( i \in \{1, \ldots, k\} \) and \( j \in \{1, \ldots, l\} \), cf. [8] Chapter 18. Based on the level of significance \( \alpha \), we can decide if our hypothesis that \( A \) and \( B \) are independent has to be rejected by considering how likely it is to obtain the calculated \( \chi^2 \) values assuming \( A \) and \( B \) are independent. In the appendix, we discuss conditions such that each \( \chi_{ij} \) can (approximately) be considered a normally distributed random variable with the expectation zero and the variance one for any \( i \in \{1, \ldots, k\} \) and \( j \in \{1, \ldots, l\} \). The mutual independence of \( \chi_{ij} \) for all \( i \in \{1, \ldots, k\} \) and \( j \in \{1, \ldots, l\} \) is discussed as well.

Next, we define a graph from the information if two random variables are independent based on the considered data. We call such a graph a dependency graph. The information of independency of two random variables can be translated into an adjacency matrix \( M \) where an entry of value one means that the corresponding random variables are mutually not independent and the value zero means that they are mutually independent. Formally for the case where we analyze the set \( X \), we define

\[
M_{ij} := \begin{cases} 
1 & \text{if } x_i \text{ is not independent of } x_j \\
0 & \text{if } x_i \text{ is independent of } x_j 
\end{cases} \tag{4}
\]

for all \( i, j \in \{1, \ldots, n\} \). Analogously, we can define an adjacency matrix for the case where we analyze the dependency of random variables to output variables in the set \( Y \) where one index of the adjacency matrix represents one input variable and the other index represents an output variable. The adjacency matrix \( M \) is symmetric since the roles of the variables in (1) can be interchanged.

Next, we discuss some special cases of stochastic independence. If a random variable is constant, we choose \( A \), then (1) is always fulfilled since \( P(A = z_A^i) = 1 \) for \( i \in \{1\} \) and \( P(A = z_A^i \text{ and } B = z_B^j) = P\left(B = z_B^j\right) \) for all \( i \in \{1\} \) and \( j \in \{1, \ldots, l\} \) because all the events \( B = z_B^j \) do not branch out due to \( A \) being constant.

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Consequently, $A$ and $B$ are independent in the case where one variable is constant. As a special case any constant random variable is independent to itself according to the definition given by (1). In contrast is a non-constant random variable to itself. If two random variables are each non-constant and identical, we denote both with the random variable is independent to itself according to the definition given by (1). In contrast is a non-constant random variable is independent to all the other variables represented by nodes of the other complete subgraphs. Consequently, each variable is independent to all the other variables represented by nodes of the other complete subgraphs. The algorithm is given in Algorithm 1.

Algorithm 1 Graph dissection algorithm

1. Sort $G$ into subgraphs: $G_c$ are the complete subgraphs and $G' = G \setminus G_c$ are the subgraphs that are not complete.
2. For $g \in G'$
   (a) Select a set of nodes $S$ of $g$ of minimal cardinality such that $g$ is decomposed into disjunct subgraphs when removing $S$.
   (b) Remove $g$ from $G'$.
   (c) Remove $S$ from $g$. Name the resulting graph $g$.
   (d) For any element in $g$:
      i. If $\tilde{g} \in g$ is complete: Add $\tilde{g}$ to $G_c$
      ii. If $\tilde{g} \in g$ is not complete: Add $\tilde{g}$ to $G'$
   (e) Stop if $G'$ is empty.

Next, we state and prove a lemma that says that Algorithm 1 is well-defined.

Lemma 1. Algorithm 1 is well-defined. That means the for-loop in Step 2 stops after finitely many iterations. The subgraphs of $G_c$ are mutually disconnected and there is a path in $G$ to any node of $G \setminus G_c$ starting in a subgraph of $G_c$. Furthermore, there is no random variable corresponding to a node of $G$ that is stochastically independent of all the random variables represented by the nodes of $G_c$.

Proof. If $G$ is a complete subgraph or consists of only disconnected complete subgraphs, i.e. $G_c = G$, then the statement is true. If a subgraph of $G$ is not complete, then there are at least two nodes that are not connected, i.e. there are two independent random variables. Let $n'$ denote the number of nodes of this incomplete subgraph. Then there exists a set of $n' - 2$ nodes that can be removed such that this incomplete subgraph decomposes in two complete subgraphs. Since there is a set of finitely many elements, there also exists a set of minimal cardinality subgraphs of $G$. Since there is a set of finitely many elements, there also exists a set of minimal cardinality subgraphs of $G$. Since there is a set of finitely many elements, there also exists a set of minimal cardinality.
that decomposes the graph upon removing it. The cardinality of this minimal set is at least one since we have an incomplete graph with two disconnected nodes and consequently we need at least a third node connected to these two nodes. Otherwise it would be a graph consisting of two disconnected complete subgraphs. Thus, we have proved that we stop after finitely many steps, since we at least remove one node from a set with finitely many nodes as long as our initial graph is not decomposed into disconnected complete subgraphs.

Since the subgraphs of \( G_c \) are disjoint per construction, we next prove that there is a path to any node of \( G/ G_c \) in \( G \) starting form a subgraph of \( G_c \). For this purpose, we consider two non-connected (non-neighbored) nodes \( s \in G \) and \( t \in G \) which always exists if the graph is not complete according to the discussion in the previous paragraph. We remove a set of nodes of minimal cardinality \( V \) from the graph such that these two nodes are each in a subgraph disjoint from each other. Then all the removed nodes were connected to both remaining graphs, which are graph \( S \) which contains \( s \) and the graph \( T \) that contains \( t \). That means there exists a path to each ever removed nodes from a remaining node. Iteratively we can consequently find a path from a node of \( G_c \) to a node of \( G \).

Next, we prove that in each iteration, we do not remove a node corresponding to a random variable that is stochastically independent of the random variables corresponding to the remaining nodes. Then, we have that there is no random variable corresponding to a node of \( G \) that is independent of all the random variables represented by the nodes of \( G_c \). Let \( V \) be a set of minimal cardinality that dissects a graph into a subgraph \( S \) and a subgraph \( T \) when being removed. If there was a node \( e \in V \) which was not (directly) connected to a node of \( S \) and \( T \) or in other words neighboring a node of \( S \) and \( T \), i.e. the corresponding random variable is independent of all the random variables represented by the nodes of \( S \) and \( T \), then this would be a contradiction to the requirement that the set of nodes \( V \) was of minimal cardinality to separate \( S \) and \( T \) since we could remove only \( V \setminus \{e\} \) which would still separate \( S \) and \( T \).

With an illustrating example, we introduce how Algorithm 1 works and motivate its usefulness. In particular, the example shows how Algorithm 1 identifies structures that variables generate that are a function of other variables. Furthermore, we compare our framework to a naive approach for identifying principle variables.

**Example 2.** We choose three pairwise stochastically independent random variables \( x_1, x_2, x_3 \) and set \( x_4 = 2v_1v_2v_3 \), \( x_5 = v_1v_2 \). The graph’s adjacency matrix is generated as defined in \( \text{[1]} \) and the graph is visualized in Figure 2.

Now, the task is to select a set of variables from which we can reconstruct the dependencies from all the variables \( x_1, ..., x_5 \).

Before the procedure of Algorithm 1 is exemplified, a naive strategy is illustrated that might be considered for the task. The naive approach for identifying principle variables starts with choosing a node randomly. Then, we iterate over all the other variables and include any variable into our set of input variables that is stochastically independent of all variables that are contained in our current set of input variables. By going through the possibilities to choose an initial node, we see that the result in this case depends on the initially chosen variable. If we take \( x_4 \) for example, no other variable will be chosen and we are not able to construct the values of the other random variables. Next, we see that the result of Algorithm 1 is unique in this case.

By Algorithm 1 we uniquely choose the set \( \{x_1, x_2, x_3\} \) as input variables which allows us to construct all the values of the remaining random variables. To illustrate the Algorithm 1, we describe how it proceeds in this example. The first set of nodes that is removed is \( \{x_4\} \), since there is no other one element set that dissects the graph upon removing it. Then only the graph consisting of \( x_1, x_2 \) and \( x_5 \) is further processed, since the graph consisting of the single node \( x_3 \) is complete. In the first graph, since it is not complete, the only node to remove to obtain two dissected complete subgraphs is node \( x_5 \). From the result \( \{x_1, x_2, x_3\} \), we can exactly construct all the other two nodes. For example, we can find the functional dependencies by regression methods staring from the variables \( x_1, x_2 \) and \( x_3 \) as the domain variables. The described procedure is also shown in Figure 3.

This example demonstrates that Algorithm 1 might be a better choice for identifying variables by which we can model all the remaining variables or predict the output of a system, respectively, than just using the naive approach introduced two paragraphs before. The reason is that stochastically independent variables are not (directly) connected to each other. The variables or functions, respectively, that are not independent of several of these independent variables link them together. Consequently these variables representing functions are likely to be removed by Algorithm 1 in order to obtain disconnected subgraphs. This leaves the real input variables left as disconnected subgraphs.
In the next step, the meaning of the complete subgraphs that Algorithm 1 returns is discussed. The complete subgraphs are the input interfaces of the dependency graph of our considered system of which quantities are measured. These complete subgraphs may be interpreted as the influx of information that propagates through the system and the values of the corresponding variables determine the values of the other random variables corresponding to the removed nodes. In the case where a complete subgraph returned by Algorithm 1 consists of only one node, we can use the corresponding random variable as an input variable for our model of the considered system. In the case where a complete subgraph consists of at least two nodes, we discuss some cases in the following on how to proceed.

Nodes of a complete subgraph correspond to random variables that are pairwise not independent. There are some cases that can result in complete subgraphs consisting of more than just one node. We discuss them in the following.

In the first case, each variable of a complete subgraph can be described by a single variable of this subgraph with a function. More specific, there exists a function to describe each random variable represented by a node of the subgraph with another random variable whose node is an element of the considered subgraph. As an example choose the dependency $x_1 = x_2^2$ as a functional connection between two random variables. Both variables are not independent of each other and this functional dependency can be described by either $x_1 = x_2^2$ or $x_2 = \sqrt{|x_1|}$. However, the square root function is not smooth considered as a function, where in contrast the square function is smooth, i.e. it can be differentiated. This can be important depending on the application of the model. For example if derivatives of the model are needed since it is used in an optimal control problem or optimization framework.
Consequently, in the case where one node of the complete subgraph is sufficient to represent all the values of the other nodes by corresponding functions, the nodes of the complete subgraph can be considered as algebraically equivalent but not analytically.

The second case where subgraphs can be obtained is that relevant variables are not measured. Not measuring relevant variables can have several reasons like that one has to decide what variables have to be recorded or measured due to limitation of storage or other lack of performance or processing power, respectively. Another reason is, that one was not aware that a variable could have impact on the description of a system or an output variables and due to limitation of storage or other lack of performance or processing power, respectively. Another reason is, that for this reason an important variable is not recorded or measured. We illustrate the scenario with the following example. Consider $x_3 = x_1 - x_2$ as a function of the mutually stochastically independent random variables $x_1$ and $x_2$. Only the variable $x_3$ and $x_2$ are measured. Since $x_3$ and $x_2$ are not independent of each other, the nodes form a complete subgraph and thus this graph is unchanged returned by Algorithm [1]. In the case that we would like to predict an output variable that only depends on $x_2$, the inclusion of $x_3$ to the set $X$ besides $x_2$ would not provide a better prediction accuracy since all the necessary and sufficient information is already contained in the variable $x_2$. In this case, the node of $x_3$ of the complete subgraph could be neglected. In the case that a desired output variable is not independent of $x_1$ (but $x_1$ is not measured), we could calculate the value of $x_1$ from the values of $x_2$ and $x_3$ by adding $x_3$ and $x_2$. Alternatively, a machine learning model could be trained and during this process the functional dependency between $x_2$, $x_3$ and $x_1$ would be implicitly learned to construct the variable $x_1$ given the values of $x_2$ and $x_3$ and then perform the prediction of the output variable. In this case the prediction is likely to perform better, if we include $x_2$ and $x_3$ into $X$. The benefit of our principle feature analysis is that the analysis for modeling can be broken down to only those subgraphs with more than one node. Only the complete subgraphs with more than one node have to be taken care of more closely depending on the purpose and required accuracy of the prediction or modeling.

However, although considering all the nodes of a subgraph, the variables corresponding to that subgraph might not contain sufficient information to make a satisfactory prediction since too many variables are not measured that are important for a sufficient prediction or sufficiently accurate model. An example can be where $x_4 = x_1 + x_2 - x_3$. If only $x_4$ and $x_1$ are measured, the nodes of $x_4$ and $x_1$ form a complete subgraph and we could for example not make a good prediction if an output variable explicitly needs the value of $x_2$, like $y = x_2 + x_3$. However, if the output variable would be like $y = x_2 - x_3$ we could make a good prediction since by subtracting $x_1$ from $x_4$ would perfectly result in the difference of $x_2 - x_3$. Consequently, if the prediction is not sufficient it may be a hint to measure more different variables, i.e. that the relevant information for the prediction or modeling is not included in the current measurements.

Summarizing, our framework can accelerate modeling since from all the variables of the total data set, which are initially all possible input variables, we extract a subset of variables. From this subset only the sets of variables corresponding to complete subgraphs with more than one node need to be further investigated to make a set of input variables from where a detailed analysis of the dynamics of the considered system can start. This analysis can be used to find the main causes or rules to predict an output variable of a system that we are interested to forecast.

In the third case, a complete subgraph can consist of many nodes. Having many nodes in a complete subgraph can be a hint that more variables should be measured. The example where $x_3 = x_1 \cdot x_2$ with the mutually stochastically independent random variables $x_1$ and $x_2$ shows that if we do not measure $x_1$ for example, the corresponding complete subgraph that Algorithm [1] returns consists of the nodes for $x_2$ and $x_3$. If in addition $x_1$ is measured, Algorithm [1] returns the two complete subgraphs $x_1$ and $x_2$ each consisting of only one node. Consequently, measuring more variables can result in complete subgraphs with less nodes each since more variables can resolve the information of the considered system more accurately resulting in more branches of the dependency graph that can be dissected.

We conclude our discussion about the complete subgraphs by showing how to approximate exact relations of variables represented by a complete subgraph. In other words, we analyze how much relevant information a variable carries with regard to calculating an (output) variable that is supposed to be modeled. The number of nodes of a complete subgraph returned by Algorithm [1] can be further reduced depending on our requirement for accuracy that we have for a model or a prediction. For example let’s consider $x_3 = x_1 + 10^{-3} \cdot x_2$ for the mutually independent random variables $x_1$ and $x_2$ with the same order of magnitude of values that $x_1$ and $x_2$ can take. Then formally Algorithm [1] returns $x_1$ and $x_2$ each as complete subgraphs. However, depending on the level of accuracy, we can find out by analytical investigations that already $x_1$ is sufficient as a model to predict or calculate the values for $x_3$. The benefit of our method is, that it reduces the variables that need to be considered for modeling or for machine learning in a preprocessing step. The preprocessing step with our principle variable analysis extracts only these variables that carry the information.

In order to find a model to describe the output variables in the set $Y$, it is not necessary to build a model and
describe the variables of $\tilde{X}$ by the ones in $X'$ and thus reconstruct all the relations in $\tilde{X}$. The relevant variables of $X'$ of which the variables of $Y$ are not independent can be analogously identified with a chi-square test as described above in the paragraphs about the chi-square test. In detail, for any $i \in D \subseteq \{1, ..., n\}$ with $x_i \in X'$, we perform a chi-square test for any $j \in \{1, ..., m\}$ with $y_j \in Y$. If for a chosen $i \in D$ for one $j \in \{1, ..., m\}$ the result of the corresponding chi-square test is that the considered variables are not independent, then we add $x_i$ to $X$ as well as all the other random variables whose representing nodes are contained in the complete subgraph where the node of $x_i$ is in due to the reasoning above in the paragraphs about the complete subgraphs starting on page 8. To investigate the connection between $X'$ and $Y$ to generate $X$, we are not limited to the chi-square test but can take any test that seems suitable to relate the variables of $X'$ not being independent of the variables of $Y$ and then apply Algorithm 5.

Example 3. We choose the following two mutually stochastically independent variables $x_1$ and $x_2$. Furthermore, we choose $x_3 = x_1 \cdot x_2$. The output variable $y$ is supposed to be only a function of $x_1$, for example $y = 1$ if $x_1$ is equal or greater a certain threshold and $y = 0$ else.

According to the presented framework first the adjacency matrix is generated for all the random variables of the set $\tilde{X} = \{x_1, x_2, x_3\}$ by the chi-square test. The graph looks like that the node representing $x_1$ and $x_2$ are connected with the one of $x_3$ and the nodes of $x_1$ and $x_2$ are disconnected. After applying Algorithm 1 to this graph, we have the set $X' = \{x_1, x_2\}$. Applying the chi-square test to identify the variables from $X'$ that are not independent of $y$, we obtain $X = \{x_1\}$ which is exactly the variable that we need as an input variable to describe $y$.

Now, we try the second procedure. If we first start with a chi-square test to identify variables from the set $\{x_1, x_2, x_3\}$ that are not independent of $y$, we obtain $\{x_1, x_3\}$. The corresponding graph is complete where the node representing $x_1$ is connected with the node representing $x_3$. Applying Algorithm 1 returns this complete graph.

Consequently, the result from both procedures are different and the procedures do not commute in general.

Based on Example 3, the following remark can be stated.

Remark 4. The process of generating $X'$ from $\tilde{X}$ and then generating $X$ from $X'$ does not commute with applying Algorithm 1 to all the variables of $\tilde{X}$ that are not independent of the output variables $Y$.

In the next remark, we describe how to find the input variables to model an arbitrary variable of $\tilde{X}$ and how to reduce an existing model.

Remark 5. We can express an arbitrary random variable $x \in \tilde{X}$ by a set of other variables based on the adjacency matrix that is constructed during the principle feature analysis as follows. From the row corresponding to $x$ of the adjacency matrix that is calculated for the elements of $\tilde{X}$ we can take all the other random variables in $X'$ which are connected to $x$. As a result there is a set of independent variables that may contain all the information of the data set to model $x$. In addition, if desired, variables that are connected to $x$ (see the row for $x$ in the adjacency matrix) but are not a variable of the set $X'$ can be taken and build a model for $x$. Using the information of the adjacency matrix is a systematic way to identify a set of independent random variables to model a certain random variable representing a quantity of a system.

Furthermore, by applying Algorithm 1 to a set of variables that are already used in a model, the necessary variables that capture all the information in the data set can be extracted and thus redundancies can be removed. However, in some cases there are pitfalls that are discussed in the following.

For example if $x_4 = x_1 + x_2 + x_3$ where $x_1$, $x_2$ and $x_3$ are mutually independent. If $x_4$ is not measured, the information contained in $x_3$ can be recovered as long as $x_4$, $x_1$ and $x_3$ are available. Applying Algorithm 1 to the set $\{x_1, x_2, x_4\}$ will remove node $x_4$ since the corresponding variable is not independent form the mutually independent variables $x_1$ and $x_2$. Consequently removing a node may cause a loss of relevant information and may result in the following. A consequence may be that modeling/prediction with the variables identified by Algorithm 1 is not sufficient, i.e. the errors between the prediction of the model and the measured data are too big for the given tolerances. This consequence can be easily checked when reducing input variables of an existing model by comparing the accuracy of the previous model with the accuracy of the model with the reduced number of input variables.

If the prediction accuracy of the model based on the new set of input variables is still sufficiently good, the previous set of input variables and equivalently the information can be recovered by the new set of input variables. The link between the old and new set of input variables consists of functional relations that compress the information necessary for the prediction. The advantage is that already existing well working models can be reduced resulting in a faster calculation of the output or a better interpretability of the total model, e.g. in terms of machine learning models.
Next, we discuss how to improve the accuracy of an existing model by adding further variables. At the same time the framework is used to reduce redundancy from the set of input variables of the considered model.

**Remark 6.** Any existing model whose predictions or calculations of output variables are considered to be not sufficient (any more), i.e. the predicted output does not fit well to the corresponding measured data, may be improved by adding further variables to the set of input variables since not sufficient information is contained within the current input variables. Consequently, supplementing the set of the current input variables with more variables that describe further quantities of our considered system may help to improve the accuracy. However, using sufficiently much of the information of a data set is just a necessary criterion for a sufficiently accurate model. The reason is that maybe not all the information to make a sufficient modeling is contained in our data set. Once the prediction based on the model with our chosen input variables is sufficient, the presented framework can be used to remove potentially existing redundancies from the set of input variables as shown in Remark 5.

Remark 6 creates awareness of checking a model’s prediction accuracy after removing each node to possibly compress an arbitrary set of input nodes in order not to lose information. The same procedure holds in principle for the case where we apply the framework to the total data set to generate a model from the scratch where there is mostly no evidence to have all the necessary variables in the data set for a sufficient prediction. The advantage of the presented framework is that it contains a systematical way to analyze when information is lost by removing a variable from the data set to obtain a purposeful set of input variables. For example each time a node is removed, it can be checked with a model if the prediction of the values corresponding to the removed nodes is sufficiently good based on the values of the variables corresponding to the remaining nodes in the considered subgraph. A model can be generated by e.g. a machine learning model which can take the action of an oracle answering the question if the prediction of the removed variables based on the remaining variables is still sufficient. If the prediction is not sufficient, the framework thus provides hints by this step by step analysis where to improve the data acquisition. For example, if the prediction of the values of a variable corresponding to a removed node is not sufficient, then removing this variable means losing information. In order to prevent this loss, it can be thought about what further variables of the considered system might be measured to improve the prediction of the variable since maybe not all effects that influence the removed variables are captured so far. However, we are aware of the fact that if a prediction is not sufficient, it does not necessarily have to mean that information is lost by removing a node. It can mean that the considered model is not suited to describe the relation between the removed and the remaining variables. For generating more confidence on this test if information is lost when removing nodes, e.g. several different machine learning models can be utilized. If at least one model has a sufficient prediction accuracy, the information in the reduced data set is adequate.

If the prediction of the output variable from the set of input variables $X$ is not sufficient, those variables could additionally be included into $X$ that were removed and could not have been predicted well by the remaining variables. An improvement of the prediction can come from the fact that not all relevant factors that influence a removed variable are captured. By including such a removed variable whose prediction was not good, we can include relevant information as shown in e.g. the paragraph starting on page 9 about complete subgraphs. However, if we have thousands of variables this procedure may not be practicable, for example since a neuronal network might not be practically trained on the many variables that are given in the beginning of the procedure. In this case, it may be easier to just measure more variables of the considered system that are not measured so far to improve the prediction. By measuring more and more variables sufficient information may be collected for an accurate prediction.

In the next example, we show that the result of Algorithm 1 is in general not unique given the same graph depending on the sequence of dissecting the graph.

**Example 7.** Let $x_1, x_2, x_3, x_4$ and $x_5$ be stochastically mutually independent random variables. However, only $x_1$, $x_3$ and $x_5$ are measured and $x_2$ and $x_4$ are not considered. We have the following dependencies $x_6 = x_1 \cdot x_2$, $x_7 = x_2 \cdot x_3$, $x_8 = x_3 \cdot x_4$ and $x_9 = x_4 \cdot x_5$. The corresponding graph and two possible ways to dissect it are given in Figure 4 where we always return a set of complete subgraphs.
Figure 4: Two possible ways to dissect a graph with Algorithm 1. In the first branch, we first remove $x_9$ and then $x_6$. In the second branch, we first remove $x_8$ and then $x_6$.

The presented framework is not limited to the used techniques as explained in the following.

Remark 8. The dependency graph does not have to be necessarily generated with a chi-square test, see Figure 1. Any test or measure that defines a dependency between two random variables is suitable. For example, we can use the mutual information between two variables [29, 39], which was introduced by Shannon [2, 12.3.3.3]. In a subsequent step, the measure of dependency has to be transformed into a statement if two variables are mutually independent. In the case of the chi-square test, there is the level of significance to evaluate if the hypothesis that both variables are mutually independent have to be rejected. In the case of mutual information, analogously a threshold has to be defined when we say that two variables are mutually independent because they have not sufficient information in common. If the measure is below that threshold, the variables are mutually independent and mutually not independent if the value is above the threshold. The threshold is necessary to filter for relations that coincidently occur on a finite data set. Analogously, we can proceed with the result of Algorithm 1. Instead of a chi-square test to find out the variables that are linked to our output variables, we can use the mutual information for example. In addition, the mutual information between the random variables can be used after a chi-square test between the variables from Algorithm 1 and the output variables. Taking only variables whose mutual information with the output variables is above a threshold can be used for model reduction via approximations.

In the next example, we demonstrate why it can sometimes be reasonable to use the mutual information test after a chi-square test in order to further reduce the model based on neglecting variables that only contribute with small effects to a model.

Example 9. Let us choose $x_1$ and $x_2$ as mutually independent random variables with values between 0 and 5.

We define the output variable $y := \begin{cases} 1 & \text{if } x_1 + x_2 \cdot 10^{-0.5} \geq 4 \\ 0 & \text{else} \end{cases}$. The variables $x_1$ and $x_2$ are the basic variables to model $y$ and the chi-square test will return both variables as linked to the output variable since this test has binary results with respect to the relation of a variable to an output variable. However, if the mutual information test is performed, the score of $x_1$ is higher of about one order of magnitude than the mutual information score of $x_2$. Depending on the purpose and accuracy of modeling, a model reduction to $x_1$ might be reasonable.

Furthermore, if it holds that $x_3 = x_1 + x_2 \cdot 10^{-0.5}$, then the output variable $y$ can be modeled by $x_1$ and $x_2$ but also just by $x_3$ if the values of $x_3$ are also given/measured. Since Algorithm 1 would always return $x_1$ and $x_2$, the number of input variables could be reduced without approximations by a detailed analysis of the dependencies of the variables returned by Algorithm 1 (the set $X'$) and the other variables of the set $\tilde{X} = \{x_1, x_2, x_3\}$. This is always the case if an output variable depends just on the projection of some variables. In our example, the projection is the sum of two variables and in addition this projection is a further measured variable in the system. Reducing the model by finding projections of relevant variables is related to feature engineering where new features are generated from original raw data by mathematical transformations like multiply each two features to obtain the value of their product.

In the first case, information is neglected and the information of the data set is approximated. In the second case the model reduction is exact where no information is neglected but presented in a purposeful representation.

In case that the dependency graph has many nodes, which means many variables are considered, calculating
the total adjacency matrix and finding a set of minimal cardinality that dissects the graph can be time consuming due to the quadratic scaling of the calculation of the adjacency matrix and the polynomial complexity for finding a minimal cut, see [13]. Consequently, in order to accelerate the calculations, Algorithm 1 can be applied to a subgraph of the dependency graph. Thus, only the adjacency matrix for this subgraph has to be calculated first in which the results of the chi-square tests for the corresponding variables are stored for later calculations. The total dependency graph is processed in parts where variables of each subgraph are removed which form a typical structure for random variables that are a function of other variables. Once no node in any subgraph cannot be removed anymore, we apply Algorithm 1 to the remaining total graph. The adjacency matrix of the total graph defined in (4) may not be complete after this procedure since chi-square tests of removed variables with remaining variables are saved. However, if we need some entries for further analysis, we can purposefully calculate them. The advantage is that we reduce the chi-square tests for variables removed within a subgraph compared to the case where we calculate the total adjacency matrix for all the nodes. In addition, sets of minimal cardinality that dissect a graph can be found faster in smaller graphs due to the polynomial scaling of the corresponding algorithm. We summarize the procedure in Algorithm 2 and call this algorithm the PFA. We call the result of Algorithm 2 the principal features.

Algorithm 2 PFA algorithm

1. Choose the maximal number of nodes \( n_s \in \mathbb{N} \) per subgraph
2. Generate disjunct sets of at most \( n_s \) nodes that cover the total set of nodes
3. Generate the corresponding entries of the adjacency matrix defined in (4) for these subgraphs if it is not already calculated in previous calculations
4. Apply Algorithm 1 to each subgraph
5. If no node has been removed from any subgraph: Consider the total graph of the remaining nodes and do Step 3 and Step 4, then Stop
6. Generate disjunct sets of at most \( n_s \) nodes from the remaining nodes and go to Step 3

In our implementation of Algorithm 2 all the remaining nodes after Step 3 are sorted in ascending order and packed one after another into sublists with \( n_s \) elements starting with the first node where the last sublist has at most \( n_s \) elements if the number of nodes is not an integer multiple of \( n_s \). Since Algorithm 2 is iteratively applied to subgraphs of the total dependency graph, Lemma 1 holds analogously for Algorithm 2. However, in the view of Example 7 the choice of the subgraphs may influence the final result, i.e. the combination of principle features.

The complexity of Algorithm 2 scales as follows. As mentioned before, generating the adjacency matrix scales quadratically and finding a minimal cut of the graph scales polynomially regarding the number of the nodes. However, by performing the calculations for the adjacency matrix just for the necessary nodes and applying the min cut algorithm to subgraphs reduces a lot of calculation effort. How much this reduction of calculations decreases the runtime depends on the particular topology of the dependency graph.

3 An evaluation of the PFA based on error identifications of a data center

In this section, we demonstrate how the PFA can be use to identify relevant variables of a data set. The data in this section is collected from a data center environment. The variables in this context describe parameters of servers and are called metrics. From this metrics the state of a server can be inferred. The information about the state can be for example used in self healing systems that automatically correct issues and thus enhance the reliability of cloud applications [6, 22]. For an efficient implementation of a self healing system, it is important to focus on the metrics containing purposeful information.

First, we describe the implementation of the PFA and subsequently show results. The implementation consists of how the data set was acquired and what programming libraries are used. The presented framework is implemented in Python 3.7. The used Python functions are specified later. In the subsequent evaluation part, the results of the PFA are compared to different strategies to reduce the data set, like the principle component analysis (PCA) [18] and a minimize redundancy maximize relevance (mRMR) method [31]. Furthermore, the post-processing of the
results of the PFA with the mutual information is demonstrated and the prediction accuracy of different models trained on the sets of input variables are presented.

The data set consists of 2154 metrics that represent different parameters of a server, see https://learn.netdata.cloud/docs/agent/collectors/collectors for a documentation of the parameters. A measurement of all the metrics at the same time point is called a data point.

Next, the acquisition of the data set is explained. The dataset used in this section was generated using 15 physical servers with identical hardware. We used a fault injection to transfer those 15 servers into a faulty state. The failures considered affect the central processing unit (CPU) and the Random Access Memory (RAM). The failure are caused by scripts that are executed on the servers. The scripts use a tool called stress (https://linux.die.net/man/1/stress) which acts as a faulty program to manipulate the percentage of CPU and used RAM. The fault injection scripts, which follow a certain structure, are shown in Algorithm 3.

Algorithm 3 Fault Injection Script

1. Initialize all 15 servers
2. Start monitoring
3. Wait some time
4. Inject fault

Initializing all 15 servers means that the script checks if it can establish a connection to all nodes in the system and if so it sets up OpenStack (https://www.openstack.org). OpenStack is a Cloud Operating System with processes for managing different parts of the servers’ hardware. Afterwards the script uploads the required shell scripts which cause the failures later on. After successfully doing so monitoring is initiated. With the monitoring tool the measurements of the servers’ parameters are done to generate the data points. For monitoring, we used a tool called Netdata (https://www.netdata.cloud). Netdata is an open-source-tool that allows us to monitor and store a server’s state in real-time. The metrics were requested and stored for each of the 15 servers each second. One failure scenario lasts 500 seconds to have sufficient time to collect data from the server in a non-faulty and a faulty state. Thus, a measurement series provides $15 \cdot 500 = 7500$ data points for each case where each data point consists of 2154 values. At the start of monitoring the script randomly waits between 100 and 400 seconds to let the system run in a non-faulty state for some time. This variation of the starting point for the fault injection results in a balance between faulty and non-faulty data points. After that time the failures are initiated remotely on all 15 servers at the same time to parallelize the data acquisition. Each data point is classified with 1 if the server was in an error state and 0 if the state of the server was error free. The starting point of the fault injection is also the point where the labels in the dataset switch from 0 (non-faulty) to 1 (faulty). Even though all 15 servers receive the same treatment, the measured results vary due to noise caused by the OpenStack processes running on them. Thereby every server provides slightly different data points. Several shell scripts able to cause CPU and RAM failures have been uploaded to the nodes. For the CPU failures, the stress tool claims a certain percentage of available processes to force the desired workload. For RAM, the stress tool allocates the desired percentage of available megabyte in memory. As Netdata not only monitors the general CPU and RAM usage but also the usage per application and user, not only two but multiple, possibly redundant, metrics change at once during fault injection.

As a measure of how many information a selection of metrics has, we use different machine learning models and rate their prediction accuracy. We use the fact that for a sufficient prediction accuracy it is necessary that the used metrics carry sufficient information regarding the prediction. We are aware of the fact that the reversal does not hold in general. A reason could be that a selection of metrics might contain all the information of a data set, however the chosen machine learning model is not a good choice for constructing the functions to calculate the relation between input metrics and output features, i.e. the prediction values. The machine learning models act as a quick test, like an oracle, answering the question if from a selection of features a sufficient prediction accuracy can be done once the model is trained on the features from the PFA.

Since the intention of the work is rather focussing on the preprocessing of data than using the processed data with various models, like machine learning models, we use the Python framework sklearn for an easy implementation of classifiers based on neuronal networks (NN) and support vector machines (SVM). The NN is implemented with the mlpClassifier from Python sklearn.neural_network and the SVM is implemented with SVC from Python svm.

In order to evaluate the prediction accuracy the r2-accuracy score (sklearn.metrics accuracy_score) is used as well as the number of wrongly classified data points from the confusion matrix.
Since the training of the NN is based on stochastic optimization methods, we perform any training and the subsequent prediction based on a feature selection 100 times. The standard deviation of the r2-accuracy score and of the wrongly classified data points is not zero. This shows the influence of the stochastic optimization routine that is used to train the NN. A further reason for performing training and prediction 100 times is that in some experiments features are randomly chosen.

The PCA is implemented with the PCA from sklearn.decomposition. A notion of the basic concept of the PCA can be found in the Related methods section.

The mRMR method is implemented with the C++ source code from [http://home.penglab.com/proj/mRMR/](http://home.penglab.com/proj/mRMR/). The basic description of the mRMR method can be found in the Related methods section. To use the mRMR method as implemented in the C++ code, a discretization of the continuous variables is necessary. The discretization in the C++ code is performed as follows. The boundaries for the bins are set by the mean ± multiples of the standard deviation (std) of the data set. We choose 1 as the maximum of a multiple of std and obtain sufficient results of prediction accuracy. Consequently, according to the description of the source code the boundaries of the bins are mean ± {0, 0.5, 1} std. When we execute the code we allocate memory for 25000 data points and 2500 variables. We use the implementation in the mutual information difference (MID) mode. This mode sorts the set of metrics such that the difference of the sum of all mutual information between the selected metrics and the output function and the sum of all mutual information among the selected metrics with each other is maximized.

Before we use the NN, SVM or PCA, the data is normalized with the MinMaxScaler from sklearn.preprocessing. This scaler is fitted on the training set and applied to the train and test set.

The chi-square test is implemented in the Python function chisquare from the Python package scipy.stats.

The data set is randomly split into a train and a test data set where we have 80% of the 30000 data points in the train data set. The remaining data points are put into the test data set. The PFA is performed on the training data set if not otherwise stated.

In this section, Algorithm 2 is used. In order to dissect the graphs with Algorithm 1 the Python routine minimum_node_cut from the Python package networkx is used. The minimum_node_cut function is a flow based algorithm to generate a set of nodes of minimal cardinality that dissects the corresponding graph upon removing this set of nodes. For details, see the documentation of networkx or [13, Algorithm 11].

The result of the PFA is further processed with a chi-square test to obtain these metrics on which the function which labels the data points depends on. The function that labels the data points if a data point corresponds to a faulty or a non-faulty state is the output function. Metrics that belong to a node of a subgraph consisting of more than one node are proceeded as follows. If the output function is not independent of one metric corresponding to the considered complete subgraph, we choose all the metrics corresponding to the current complete subgraph for the selection of the relevant input metrics. For the reasoning, see the paragraph starting on page 8.

For further model reduction, we determine the mutual information of each metric with the output function and take only the metrics above a certain threshold $\theta > 0$. The threshold $\theta$ is specified for each experiment, see e.g. the experiment whose results are presented in Table 2.

Next, it is explained how we use the PFA for the analysis of the data set introduced above. For the binning, i.e. the discretization of the co-domain of the random variables, we use Algorithm 4 with $\nu = 500$. By the choice $\nu = 500$, the chi-square test had at least 5 data points for each expected frequency of the joint outcome of two metrics in any calculation, see Remark 13 for details. For any chi-square test in this section the hypothesis that two variables are independent is rejected on a level of significance of 1%. This level of significance is a common choice and provides reasonable results as well in the following of this section. Next, Algorithm 2 is used with $n_s = 50$. We experimented that the subgraphs in this section consisting of at most 50 nodes can be processed in reasonable time from the minimal_node_cut function.

The experiments are performed on a laptop with a 2.3 GHz 8-Core Intel Core i9 processor with 32 GB 2667 MHz DDR4 memory. The time needed for one run of the PFA with the settings discussed in the previous paragraph on this laptop takes about 4 minutes.

Our first experiment is performed as follows. On the train data set the PFA extracts 206 metrics. In order to compare the prediction accuracy of the NN and the SVM with regard to different selections of metrics the mean values of the r2-accuracy score and the mean number (\#) of wrongly predicted data points are given in Table 1 with the corresponding standard deviations (std) from 100 training and subsequent prediction sweeps. The results of the NN and the SVM based on these 206 metrics after the training on the train data set and the subsequent prediction on the test set can be seen in Table 1 first and second column. In comparison, the NN and the SVM are trained on randomly chosen 206 metrics that are non-constant, third and forth column. There are 1536 non-constant metrics in the data set. Non-constant means that there is a measurement of this metric which is different from the other ones. In the fifth and sixth column of Table 1 there are the results where the NN and the SVM are trained on all
the non-constant metrics.

|                  | PFA NN | PFA SVM | random NN | random SVM | all NN | all SVM |
|------------------|--------|---------|-----------|------------|--------|--------|
| r2-accuracy mean | 0.9973 | 0.9982  | 0.9875    | 0.9580     | 0.9932 | 0.9663 |
| r2-accuracy std  | 0.0029 | 10^{-16}| 0.0179    | 0.0207     | 0.0102 | 0.0    |
| # wrongly classified mean | 16.2 | 11.0 | 75.3 | 251.97 | 40.9 | 202.0 |
| # wrongly classified std   | 17.7 | 0.0 | 107.7 | 124.4 | 61.2 | 0.0 |
| time of training mean     | 8.4584 | 3.9269 | 12.7301 | 5.2470 | 32.5983 | 25.4406 |
| time of training std      | 1.7704 | 0.2962 | 3.7647 | 2.6496 | 3.5409 | 0.6769 |

Table 1: Statistics for different methods of the selection of the input metrics for two different models. The first model is a neuronal network (NN) classifier implemented in mlpClassifier of sklearn. The second model is a support vector machine (SVM) classifier implemented in SVM of sklearn. In the column PFA NN and PFA SVM there are 206 metrics selected with the PFA on which the training is performed. In the column random NN and random SVM there are 206 randomly chosen metrics from all the non-constant metrics of the data set on which the training is performed. In the columns all NN and all SVM, the models are trained on all the non-constant 1536 metrics of the data set on which the training is performed. In the last two rows there are the mean and std time in seconds to train the corresponding model on the chosen metrics.

The results of Table 1 can be interpreted as follows. In the case where the metrics are selected from the PFA, the NN and the SVM perform equally well. In the case of fixed metrics and the classification by the NN, i.e. the columns named with PFA NN and all NN, the std is greater than zero. This comes from the stochastic training method. We assume that the reason why the performance on the PFA metrics is better than on all the non-constant metrics is that small models are easier to train. Since the information is concentrated in models using just the relevant metrics, the method can easier distinguish if a small progress in learning is due to an already optimal trained model or if only few weights of the model change since only a little number of metrics is linked to the output variable and thus only these linked metrics change during learning anyway. Illustratively spoken, the information from the PFA is concentrated and not diluted. In comparison to the case where the 206 metrics are chosen randomly, we see that the metrics chosen with the PFA framework perform much better. Summarizing Table 1 the learning on the PFA selected metrics works better and faster than on all the other two cases independent of the considered machine learning model.

There are high accuracy scores for the NN and the SVM, see Table 1 in any cases. Consequently, we are confident that the corresponding prediction function can be well approximated by the chosen models. We summarize that the PFA provides metrics that contain sufficient information from the data set for the prediction if a server state is faulty or non-faulty.

Next, an NN and an SVM is trained each 100 times on a set that is transformed with the PCA providing 206 components carrying 99.7252% of the variance of the original data set. The NN has an r2-accuracy mean of 0.9983 with std 0.0002 and 10.25 wrongly classified data points with std 0.1645. The needed time for a training is in mean 3.3380 seconds with std 0.1645 seconds. The SVM has a mean r2-accuracy score of 0.9674 with 0.0001 std and 195.49 wrongly classified data points with 0.6707 std. Since the NN prediction accuracy based on the PCA is comparable with the prediction accuracy of the NN based on the PFA, the data set transformed with the PCA contains the necessary information for learning the function for the prediction if the server is in a faulty or a non-faulty state. However, there is a difference in preprocessing data sets with the PCA and the PFA. The PCA determines a linear combinations of the original features to transform the data set into a new data set where the new features are the linear combinations of the original features. The PFA extracts the features from the original data set that carry the relevant information. In the presented example the SVM cannot learn from data set transformed with the PCA as good as on the original features presented from the PFA. From the point of training a machine learning model the PCA and the PFA might be considered equally. From the point of modeling and interpretability, the PFA has the advantage of providing a set of input features of the original set from where the modeling can start. To start from the original features can enhance the interpretability of the model. The PCA linearly transforms the original features into a new data set. For this transformation all the original features may be needed. In case of the PFA, all the features that are not returned as relevant may be neglected and do not need to be measured when applying the model in a use case. Furthermore, learning on the original data set may provide advantages for explaining the models.

Since from Table 1 we can extract that the NN and the SVM perform equally well on the PFA metrics and the NN performs better in the non PFA cases, the remaining part of this section is carried out with the NN if not otherwise stated.
Next, the mutual information of the 206 metrics from the PFA and the output variable (function that labels if a data point is from a faulty or a non-faulty server state) are determined. Then only the metrics that are above a certain threshold $\theta$ are chosen. We take $\theta \in \{0.05, 0.1, 0.15, 0.2\}$ as a reasonable selection where the effect of approximating information can be seen quite well. Analogously, each experiment is performed 100 times and the resulting statistics of the experiments are presented in Table 2. If the metrics are randomly chosen, new metrics are selected after each sweep.

| r2-accuracy mean | r2-accuracy std | # wrongly classified mean | # wrongly classified std |
|------------------|-----------------|--------------------------|-------------------------|
| PFA 0.05 140     | 0.9981          | 0.0003                   | 10.9                    | 1.8                      |
| rand 140         | 0.9813          | 0.0210                   | 112.3                   | 126.0                    |
| PFA 0.1 122      | 0.9979          | 0.0020                   | 12.4                    | 11.8                     |
| rand 122         | 0.9772          | 0.0327                   | 136.6                   | 196.4                    |
| PFA 0.15 114     | 0.9973          | 0.0003                   | 16.2                    | 2.1                      |
| rand 114         | 0.9772          | 0.0252                   | 136.6                   | 151.3                    |
| PFA 0.2 107      | 0.9189          | 0.0018                   | 486.4                   | 11.1                     |
| rand 107         | 0.9774          | 0.0281                   | 135.6                   | 168.3                    |

Table 2: Number of metrics that are further reduced by taking only the metrics whose mutual information with respect to the output variable are above a threshold $\theta$. In the row starting with PFA, we have the results of the selection of variables after the PFA and $\theta$ equaling the number following PFA. The number that follows is the number of metrics from the PFA that are above the corresponding threshold and are used for a prediction. In the subsequent row starting with rand the experiment is performed on randomly chosen metrics where the number of used metrics equals the subsequent number.

In Table 2, the prediction accuracy of the selection of variables whose mutual information with respect to the output variable is above $\theta = 0.05$ increases compared to the model learned from all the 206 variables from the PFA of Table 1. A reason might be that the smaller model can be trained easier and that this advantages predominates the fact that information is deleted from the data set. A further reason can be that variables are removed that might be selected by the PFA due to spurious correlations which coincidently may exist in our data set. If we proceed, the prediction accuracy decreases since more and more metrics that are relevant for the prediction are neglected, see the column r2-accuracy mean of Table 2. Since the PFA selects metrics such that the redundancy is removed, we cannot construct information once deleted by the other metrics. For the case of $\theta = 0.2$ much relevant information is deleted since the randomly chosen metrics perform better. Further the relative small std of wrongly classified data points may be an indicator that the misclassification is due to a systematic loss of information that is caused by the successively reduction of number of metrics.

In order to demonstrate that focusing on the metrics with the highest mutual information with respect to the output variable, does not necessarily provide the best results, we perform the following experiment. We take the mutual information of all metrics with respect to the output variable and choose the metrics whose mutual information is above the threshold $\theta = 0.7752$. This threshold provides 208 metrics. We perform the training of the NN on these 208 metrics 100 times and obtain a mean r2-accuracy score of 0.9102 with a standard deviation of 0.0164 and a mean of 510 with std of 98 wrongly classified data points. Again there is a small std. This may indicate that information is systematically missed. The reason is that there is now a high redundancy within this set of input variables but this set does not cover the total information necessary for a sufficient classification. The result is that just taking variables that have a high mutual information score is not sufficient for a good prediction since the input information is not necessarily independent and thus may contain redundant information instead of the total information of the data set. This demonstrates that also many metrics with each only a small contribution of mutual information with respect to the output variable can make a valuable contribution to a correct prediction. An illustration is a function that depends on many variables. If each variable has the same mutual information score with the function, the score of each variable decreases the more of such variables the function depends on. By just focussing on a threshold of mutual information, many variables of one function can be deleted. Consequently for a model reduction it is not always the best to focus just on metrics with the highest mutual information since the interplay of metrics with only a little mutual information each with the output function can be important. The discussion of this paragraph shows that reducing the variables with the PFA is a good way to end up with metrics being relevant for a prediction since the prediction accuracy of Table 2 is much better than by choosing the metrics with a single mutual information test.

Next, the PFA is compared with the mRMR method on the data set that is used for the experiments presented
Table 3: Results from the mRMR method for different number of metrics to be selected denoted in the columns. In the rows the mean classification accuracy of the NN and the SVM are presented. Furthermore, the mean training time in seconds (s) for the NN and the SVM is given.

| metrics | 150 | 175 | 206 | 230 | 300 | 350 |
|---------|-----|-----|-----|-----|-----|-----|
| NN mean r2-accuracy | 0.9426 | 0.9987 | 0.9990 | 0.9990 | 0.9958 | 0.9905 |
| NN mean # wrongly classified | 344.18 | 7.77 | 6.17 | 6.11 | 24.73 | 56.75 |
| NN mean training time (s) | 12.27 | 9.74 | 10.32 | 7.72 | 11.27 | 12.07 |
| SVM mean r2-accuracy | 0.9422 | 0.9985 | 0.9985 | 0.9985 | 0.9985 | 0.9663 |
| SVM mean # wrongly classified | 347.0 | 9.0 | 9.0 | 9.0 | 7.0 | 202.0 |
| SVM mean training time (s) | 1.86 | 1.77 | 2.37 | 2.27 | 3.22 | 3.91 |

in Table 1 For the purpose of comparison a different number of features is extracted by the mRMR method and a classification with an NN and an SVM is performed on the same data set as used for the experiment where the corresponding results are presented in Table 1. The training and subsequent prediction is performed on each set 100 times. The results are presented in Table 2 The fact that the intersection of the 206 PFA metrics with the 206 mRMR method metrics consists of only 22 common metrics shows that both methods work differently. The aim of the PFA is to find the arguments in data sets with which a considered function can be modeled. The aim of the mRMR method is to find a set of metrics that provides the best prediction accuracy where the different metrics in this set are supposed to be as mutually independent of each other as possible. The mRMR method does not necessarily distinguish between features that are functions of others and the corresponding arguments. If an output function depends on projections of features rather than on the metrics explicitly, the mRMR method is likely to choose the features that represent the projection. For example in a data center the CPU utilization depends on the sum of all the CPU utilization of any process that is running in the data center. If an output function just depends on the sum of the CPU utilization the mRMR method is likely to pick the metric describing the total CPU utilization instead of the metrics describing the single CPU utilization of any process running in the data center which is more likely using the PFA. In Table 3 we see that the prediction accuracy sharply improves when taking more than 175 metrics. The results in Table 1, Table 2 and Table 3 show that both methods work successfully. Both methods can provide useful sets of metrics from where a modeling can start. We remark that the number of 206 metrics obtained from the PFA and possibly needed to describe the label function well in this case is a well working initial guess for the number of metrics the mRMR method is supposed to return. To obtain the 206 metrics from the used implementation of the mRMR method, it took about 2.5 hours and about 5 hours to obtain 300 features.

The prediction accuracy in Table 3 improves beyond 206 metrics. This improvement can be explained as follows. As discussed e.g. after Remark 6 removing a feature that is a function of other features can cause a loss of information if not all arguments the function depends on are contained in the considered data set. The mRMR method includes step by step any feature that shares mutual information with the output function and that has as little mutual information with the already selected features as possible. It can happen, if the number of features to be selected is sufficiently high, that also features being functions of features are selected in the cases where arguments of the function are missing to increase the amount of information in the set of selected features. However if the selected features exceed a threshold, the gain of further information by the additional features is small and wasted by computational issues as discussed in the paragraph starting on page 10. The inclusion of features that are functions may be desired if the focus is on compressing a data set to obtain the best prediction possible. However, in the case where the focus is to analyze the relations within a data set, having features that are functions in the set of independent arguments may be undesirable since the aim is to find basic features with which all functions can be constructed to understand the relations and dynamics how the dependent features evolve given the input variables. In this case, it can be helpful that we are made aware by a not sufficient prediction accuracy that the data set is missing some further relevant features that should be included.

In the following, we discuss how to make the PFA robust with respect to the data set’s statistic properties upon interchanging parts of the data, i.e. by making new train data sets. For the next experiment, the train data set is reduced to 95% of the data. The data points to be left out are chosen randomly. The sampling of new data sets with 95% of the original training set is performed 5 times. The sets of the metrics returned by the PFA on each data set are intersected. Subsequently, 161 common metrics are obtained. The training and the prediction of the NN is repeated analogously as described above 100 times on the original train and test data set. We obtain the following results. The r2-accuracy mean is 0.9984 and the std equals 0.0022. The mean of wrongly classified data points is 9.71 and the std is 13.1044. If the 182 metrics are used that we obtain from the PFA after applying it to the total data set (joining train and test data), the corresponding r2-accuracy score is in mean 0.9945 and the std is 0.0036.
Th mean of wrongly classified data points is 33.1 and the std is 21.8. We interpret this result as follows. Strong dependencies and the corresponding stochastic properties are robust with respect to interchanging data points. However, relations that are only coincidentally in a data set are not robust with respect to interchanging data points. As experienced in this case interchanging data points can significantly change the stochastic properties of some parts of the data. On the other hand, there are relations that are robust with respect to interchanging data. This relations are extracted with the PFA and a sufficient prediction is possible as the results indicate. Consequently, by using the intersection of the sets resulting from the application of the PFA to different splittings of a data set extracts the strongest dependencies that are likely to be non-spurious relations between the corresponding metrics. Hence, the signal-to-noise-ratio is improved enhancing building significant models. In the case that instead of the PFA the PCA is used on the train data set, used for the experiment presented Table 1, to extract 161 components carrying 99.5679 % of the variance of the data, we obtain a mean r2-accuracy score of 0.9983 with 0.0002 std and a mean of 10.24 wrongly classified data points with std 0.9287. The mRMR method provides a mean r2-score of 0.9986 with 0.0003 std and 8.61 mean wrongly classified data points with 1.9692 performing the training and the prediction 100 times on the train and test data set as used for the experiment presented Table 1. The variations of the results of the mRMR method regarding performing it on different slightly varied data sets (90% randomly selected from the train data set) is small. Only the positions of the single metrics in the returned lists slightly differ sometimes. Consequently, the intersection of these lists contains almost all the metrics of the results up to 2 metrics considering lists of 200 metrics from 3 sweeps.

A related experiment to the experiment from the last paragraph is the following. The samples in Step 2 of Algorithm 2 can be sampled randomly instead of generating the sub sets of nodes by dividing the ascending sorted list of nodes by packing \( n_s \) nodes one after another into a list. For each experiment with randomly sampled sub sets in Algorithm 2, the results of the PFA slightly differ in our three runs of the PFA. The number of selected metrics is between 192 and 199. Possible reasons for the slight variation are discussed on page 8 ff. The sets of metrics, including the set that we use for the experiments above with the 206 metrics, are the same up to about 20 variables. We train an NN and an SVM model on each set 100 times and obtain the following mean values. The r2-accuracy score for the NN model ranges between 0.9929 and 0.9988 with std 0.0013 and 0.0076. The wrongly classified data points range between 7.27 and 42.55 with std 7.5404 and 45.7957. For the SVM, the r2-accuracy score equals 0.9985 and the wrongly classified data points are 9.0 in any case. If an SVM model is used, the results on the used data set indicate that the SVM model is not sensitive to small variations of the result of the PFA.

We can summarize the last two paragraphs as follows. It can be a possibility to perform the PFA on different randomly sampled train data sets and let the samples in Step 2 of Algorithm 2 be selected randomly. On any result of the PFA machine learning models can be trained and we can choose the set of input metrics with the best prediction accuracy. This result can be compared to the result that is obtained when sampling randomly different train data sets, perform the PFA on each data set and intersect the results.

In the next experiment, we investigate the PFA on different splittings of our total data set starting with 80% of the total data set and decrease the part of data points that is interchanged in each experiment to test if there is a threshold when the stochastic properties of the data set are robust with respect to interchanging data. For this experiment, we join the training and the test set and split the total data set in randomly chosen train and test sets with a certain percentage of data points for the train data set. We repeat the procedure five times with the same ratio of elements in the train and test data set. The metrics that are obtained are compared if in each of the five sweeps the result of the PFA is the same. This is the case if we only interchange 0.1% of the total data set. We remark that this robustness how many percentage of the data points can be interchanged until the results of the PFA change is a property of the data set.

The framework can module wise be applied to analyze relations of coupled systems as described in the following remark.

**Remark 10.** Once the metrics are identified that are related to model an output function, e.g. a function that labels measurements, we can interpret the identified input metrics in turn as functions that are influenced by external processes that are not contained in the current data set. An example can be processes running on a server. Then corresponding measurements can be performed resulting in a data set containing the values for the new output functions and processes running. This set is analyzed with the PFA to obtain the new input variables, e.g. the processes that are related to the new metric output variables. Iteratively, we can build a model for any subsystem. Thus we can glue these well validated submodels together via the corresponding input and output functions to built a total model module wise. For a data center example it means that once the internal processes are understood, it can be investigated what external processes influences the internal processes. Thus further explanations can be found on how an error of a server may be caused by a process. Of course, if we are just interested which processes are involved in error causing events, the intermediate step via the metrics is not needed. However, this demonstrates
how the presented framework can be used to analyze the relations in a complex system step by step and how well validated submodels can be recycled to answer future research questions instead of starting for any issue with a new model from the scratch.

4 Application of the PFA to a single cell data set

This section is intended to show the usability of the PFA in biology. In particular, to analyze gene expression profiles of different cell types. The features in this scenario are the expression levels of the different genes. With the opportunity to measure the expression patterns of single cells, each of such a cell measurement is a data point that provides the values for the features. On each of a data point a corresponding output function can be defined, like a label for the corresponding cell type from which the data point is measured. Such cell types can be a tumor cell or a physiological cell of tissue. Further, a stage of a stem cell in its maturation process and a corresponding differentiated cell type. Once an output function is defined on the data points, the PFA may return a set of genes that carries the information to construct this function. Thus two different cell types could be distinguished from their expression levels of the relevant genes. Starting from these relevant genes, we can build a model to analyze what alterations of gene expressions are responsible to transform one cell type into another for example.

The data set from the presented example contains different expression patterns of macrophages from mice. The GEO data set with the accession number of GSE134420 were downloaded under https://pubmed.ncbi.nlm.nih.gov/31391580/, among them one sample SIA0 (accession number: GSM3946323) was extracted. The file begins with the barcodes of each cell and contains the ribonucleic acid (RNA) count of each cell and gene. The RNA count is the number of RNA molecules that are transcribed from a gene corresponding to the expression level of each gene.

The data was carefully processed using Seurat package 11 (version 3.2.0; https://satijalab.org/seurat) as follows. The low quality cells, including broken cells with unusual high percentage of mitochondrial gene expression (>7.5) and low expressed gene features (<200) were firstly excluded from the data set. After a global-scaling normalization based on the top 2000 variable gene features, 15 principle components were selected to calculate the distance and find the neighbors. A resolution parameter of 0.5 was then applied to classify these cells into 7 big clusters and 1 small cluster (n<50). Annotation using gene markers, naming the 7 big clusters, resulted into three clusters and 1 small cluster (n<50). Annotation using gene markers, naming the 7 big clusters, resulted into three clusters and 1 small cluster (n<50). Annotation using gene markers, naming the 7 big clusters, resulted into three clusters and 1 small cluster (n<50).

The gene expression pattern normalized with the transformation $x \mapsto \ln (x + 1)$ was exported into a matrix for further analysis. The normalized expression pattern of each cell is labeled according to which cluster a cell belongs.

Instead of labeling the measurements by clustering the measurements with Seurat, the labels can also be directly measured if the cells can be sorted according to certain properties, for example with a fluorescence-activated cell sorting 32.

We choose the cluster with label 1 (CX3CR1, interstitial macrophage) and the cluster with the label 3 (lining macrophage). The processed data set that we use in this section has 9513 different genes and 121 data points. The 121 data points consist of the cells of the two clusters where the number of cells that belong to a corresponding cluster is almost equal.

The implementation of the PFA is the same as in Section 3. In the current section, it holds $\nu = 25$ in Algorithm 4. With the choice of $\nu$ no expected frequency in the chi-square test is below 5 data points.

For the training of the machine learning models, the data is split randomly into a train and a test data set where the train data set contains 80% of each class of the labels of the total data points.

The PFA analysis takes about 75 seconds and returns 9 genes. The NN and the SVM are trained each 100 times and subsequently predict the cell type of a data point of the test data set depending on these 9 genes. The results are presented in Table 4. The discussion of the results is analogous to the ones of Table 1. The results in Table 4 demonstrate that the PFA can also work on small data sets like the one used in the presented case consisting of only 121 samples. Moreover, the results show the benefit of a preprocessing and an analysis of the data set before building models when comparing the prediction accuracy on all and the 9 genes. We can summarize that in the presented example the selection of the PFA contains sufficient information to model the difference of the two cell clusters.

The results from the PFA can also be validated from a biological perspective. The 9 genes are denoted with Agfg1, Slc50a1, Msn, Sup5, Dhdds, Pih1d1, H2-Ob, Rps14, Atic in the data set. These genes indicate the difference between the interstitial macrophage and lining macrophage with regard to a specific metabolism induced by Rps14, Slc50a1, Atic and Dhdds, antigen processing (H2-Ob) and cell proliferation/migration regulated by Msn. The PFA offers a rapid way to understand the new features of novel-reported cell subtypes, for instance in this case, the epithelial-like lining macrophage which forms an internal immunological barrier in the synovial lining. Compared
to regular differential gene expression analysis, the PFA offers efficiently an augmenting view to understand the differences regarding features between cell types.

We conclude this section how the PFA can be further used to analyze cell behaviors and the causing relations for the behaviors module wise.

Remark 11. The PFA can be used to identify genes or proteins from where an output function, e.g. a label of cells, can be modeled. Subsequently these identified genes or proteins can in turn be defined as output functions that are supposed to be modeled by different input variables or features, respectively. For example the expression pattern of these genes can be measured as well as external stimuli in the environment of the cell, like concentration of hormones or other signal molecules. Then the PFA can be applied to find out the external stimuli that effect the corresponding genes. By iterating the process of modeling former input variables with related other submodels, we can build a total model from submodels by glueing them together via defining input-output-interfaces. The PFA framework can help to analyze the data and identify the relevant parameters for each submodel. By breaking a system into subsystems, we obtain building blocks of understandable subsystems revealing the driving causes for a behavior of a system. Moreover, the well validated submodels can be recycled for new research questions without starting from the scratch. An example can be the communication of immune cells. Once an immune cell type is modeled regarding what signal proteins it secretes upon certain stimuli, a model of the total immune system can be modeled from the models of several different immune cells.

The next remark is an example where an output function represents continuous values.

Remark 12. In biology, the t-distributed stochastic neighbor embedding (t-SNE), which is an unsupervised machine learning method, is used to projected single cells into a plane according to their expression pattern \[21, 46\]. With this method the cells can be clustered and the clusters can be visualized. In order to study what genes contain the relevant information for the clustering of the t-SNE, the PFA can be used as follows. Each cell that is projected into the plain can be characterized by a two dimensional vector representing the coordinates of the cell in the plane. This vector-function is defined as the output function. The PFA is now used to find the genes that are the arguments of this function that maps the coordinates of each cell into the plane. By focusing on the relevant genes that are responsible to infer the position of the cell in the plane, a model can be worked out that describes how to influence which gene to reproduce the observed transformation of the cells. Illustratively spoken, the PFA can be used to learn from unsupervised methods and subsequently transform this information into a mechanistic model.

5 Related methods

In this section, we discuss the relation of the presented framework to other already existing methods to preprocess data sets and extract relevant variables from data sets or reduce a data model.

There are other methods to reduce the dimensionality of a data set by compressing the information of the total data set. For example the principle component analysis (PCA) \[18\] decomposes a data set into a linear combination of the principal axes. However, it is challenging for the PCA to model non-linear relations between the variables. In the linear case, we may obtain a transformation of the data set that can be described with less variables. These variables are linear combinations of other variables from the original data set and it may be challenging to interpret these new compound variables.

Furthermore, there are rank correlation methods like, Spearman’s or Kendall’s test, see \[47, 37\]. These methods can be used instead of a chi-square test, see Figure 1 to evaluate if two variables are independent of each other. A threshold defining independency needs to be defined, as discussed in Remark 8. However, for the rank correlation
methods, it is challenging to detect non-monotonic relations between variables. The application of e.g. a chi-square test does not have limitations concerning functional relations of variables. In cases where a rank correlation methods is better suited to analyze the dependencies of the features, we can use the presented framework to compress the information of independency from the rank correlation methods as summarized in Figure [1] where the chi-square test is replaced by a corresponding rank correlation method. Subsequently, the correlation between the features can analogously be modeled into a corresponding dependency graph by defining thresholds for no correlation of two features and the workflow is as depicted in Figure [1].

If techniques from non-linear systems identification like the FROLS algorithm, see [2] for details, are applied, we need to specify the terms of which the model is supposed to be generated. These models can be polynomials of the variables for example. On the one hand, these polynomials can result in an enormous growth of parameters for all the monomials to capture all the combinations of variables. On the other hand specifying a model is not necessary if the model is supposed to be learned by a machine learning algorithm. The fit of a polynomial model by e.g. regression can be applied after the application of the PFA just for the identified relevant variables.

A similar problem may be faced if we have to choose kernel functions to project non-linear dependencies of random variables to linear relations [24]. In this case, we have to make assumptions on the considered data by choosing a kernel in contrast to the presented method where dependencies are analyzed without a previous assumption on the functional structure of the model.

There is a technique from neuronal networks, called autoencoder [30], that compresses the information of input variables to a smaller set of variables. However, the autoencoder needs to be trained on the total data set, where we might have the curse of dimensionality. The PFA is a tool to prevent this situation. Moreover, if the autoencoder is trained, it is challenging to understand how the neuronal network compresses the information of the data set and what the meaning of these compressed output nodes, which are the input nodes for the modeling, is. In particular, it is also challenging how the total data set is related to the output nodes of the autoencoder. Consequently, it may be hard to find out, if or which variables of the total data set are necessary for the prediction anyway and which can be neglected.

Another method of feature selection is to select a subset of features and train machine learning models on this selection. Finally, the selection of features is chosen that provides the best accuracy of prediction. This method of feature selection cannot be applied when there is a large number of features due to the combinatorial effort. The PFA returns features corresponding to complete subgraphs. Proceeding like in the paragraph starting on page 9 only subgraphs are returned where there is at least one feature of which the output function is not independent. Since the features corresponding to different complete subgraph are independent and thus represent information that is not redundant, the procedure of combing different features can remarkably be simplified. We choose a subgraph and train a machine learning model on any combination of the features corresponding to the chosen subgraph while we take all the other features that do not correspond to the chosen subgraph but to the other features returned by the PFA framework. We choose the combination of features that provided the best prediction accuracy. If two selections are comparable, then we choose the one with the smaller number of features. Then we proceed in the same way with the next complete subgraph that has more than one node. The PFA structures and thus reduces the possible combinations of features to only a few number such that a fine tuning of a feature selection can be performed by trying any combination. A discussion why the complete subgraphs with more than one node can correspond to features that can be possibly sorted out is from page 8 to page 11.

A class of methods for constructing causal networks are causal inference methods, see [7]. This class of methods uses the conditional independence of random variables and subsequently relates this conditional independence information in a graph, namely a directed acyclic graph (DAG). Going through this graph in the direction of the edges, starting from the nodes that do not have an incoming edge (input nodes), can be interpreted as giving explanations for the subsequent nodes in the sense that one quantity is the cause for alterations of the other quantity represented by the corresponding node. The causal inference methods and the PFA can be combined as follows. Since the main intention of the PFA is to identify functions of features and thus compress the information of a data set to the essential argument features, the application of the PFA is in particular useful in large scale problems to reduce the feature set where there are many features and possibly more than one output function. The reduction to the main features may save a lot of combinatorial calculation effort. One possible combination of both methods is that the PFA can be used to provide the input nodes from which the DAG can be constructed by a causal inference method. The PFA can thus provide a reasonable procedure to give roots from where a reasoning of a causal inference method can start. This may also be an opportunity to obtain some reasonable initial nodes from where to start creating a DAG again if the output from a causal inference method is challenging to interpret. A further possibility to combine both methods is where we would like to find the essential model to calculate/predict output variables and would like to have some features in between the input and output variables. This can be useful
to better understand the function that maps input variables to output variables. For the described application we proceed as follows. Once we have the input variables by the PFA, all the other features that are stochastically independent of the output variables are sorted out. Then we can apply a causal inference method to construct a DAG as an explanation going from the input to the output nodes. This may save calculation time since the feature space can be considerably reduced.

An analogously discussion as for the interference methods holds for methods building association rules for a data set, see [16] Chapter 6 and Chapter 7. Association rules describe conditions (values that features have) that lead to the outcome of another feature with conditional probability.

We would like to remark that finding a causality may not always be the focus of modeling. For instance, if the statement “condition 1 and condition 2 is true” be equivalent to “condition 3 is true”. Then we could say that condition 1 and condition 2 cause condition 3 since no other conditions influence condition 3. In the case that condition 3 is a disease, we usually would like to know the causes. However, since we have the data available for all the three conditions, maybe for some use cases, it is also interesting to build a model to infer condition 2 from condition 1 and condition 3, not as a causal model but just exploit functional dependencies to infer a quantity from others, e.g. to infer something about the causes given the effects. An analytic example is where \( x_1 = 2x_2, x_2 = 3x_3 \) building a complete subgraph. As discussed for the complete subgraphs, see page 8 ff., it depends on the context which variable to take to describe the other variables and thus exploit the functional information in the data set. The PFA can be used both in the causal case and the non-causal case. However, when using the PFA, a decision which variables to model by which variable, sometimes has to be made, see Remark 5. The reason is that the functional relations, which the PFA identifies, is more general then a causality which is a special functional relation. The PFA structures the relations within the data set and breaks the total data set down to subsets on which decisions can be clearly made if necessary.

Two interesting use cases of the discussion of the last paragraph is the following. The PFA alone or combined with a causal inference method can help to build the topology of a Bayesian Network [28], in particular in large scales. The topology is basic to calculate the distributions of events of an observed system to infer causes for outcomes of random experiments. A second example is generating the topology of gene regulatory networks that are introduced in the introduction.

Furthermore, the PFA can analogously be applied to the linear and non-linear Granger-causality [14, 17, 43]. The Granger-causality is a framework to investigate if time series can be predicted from its own history or if there is a better prediction with the inclusion of the history of the time series of other quantities. From the causality information a graph is generated. The PFA can be applied to the causal information graph when we convert the causal information graph into a dependency graph by replacing any directed edge with an undirected edge to investigate large scale graphs for instance to obtain extra insights into the relations. From the PFA resulting variables all the removed variables may be modeled. While Granger-causality is a concept explicitly for time series data, the PFA can be applied to both time series data and to data where the timely relation of the data points is not given as shown in the present work. The PFA identifies the features that are functions of other features. A functional dependency between features also includes the case where a feature reacts time delayed to another feature which we may call a causal relation. A feature that reacts time delayed to another feature can be modeled as a composition of functions. This composite function is a function with a delay function in the function’s argument modeling the time shift.

The PFA is similar to the class of methods minimizing redundancy maximizing relevance (mRMR) [31, 12, 34, 15, 3, 20]. The basic concept of mRMR methods is to find a selection of features that is most relevant to an output function, meaning that the information of the feature is well suited for a prediction of the output variable, and at the same time that the features within the selection are minimally redundant to each other feature in the selection, meaning that the information to predict a feature from a different feature in the selection is small. To describe the relevance and the redundancy of features different scores, like the mutual information, are defined. Any selection of features can be mapped to these scores and the selection is optimized with regard to these scores. Consequently, the mRMR methods need to solve (non-linear) integer optimization problems. The difference of the PFA to the mRMR methods is that the PFA does not optimize a selection of features with respect to analytical scores. The PFA uses algebraic information from an independency graph resulting from a binary test if the hypothesis that features are independent of each other has to be rejected to identify features that are functions of others. As discussed in Remark 5 the graph can be generated from any score that measures the relation of two features. Consequently, the algebraic information of the dependency graph can be combined with existing mRMR methods to accelerate the solution of the corresponding integer optimization problems which often suffer from a challenging scaling. A possible strategy can be to apply the PFA to dissect the dependency graph to a certain degree and then apply an mRMR method to these disjunct subgraphs. The results from each subgraph are independent based on the used
score or test of independency. Thus the results from each subgraph can be joined without touching the redundancy of the total set of selected features. The aim of the PFA is to delete all the features that are functions of other features and thus to leave only the independent features that are the arguments of all the functions. The arguments can be used to model the dynamics of the data set or the features corresponding to the arguments can be further reduced by picking only these features of which output variables are not independent. Consequently, the procedure of the PFA framework is an alternative method to the mRMR methods to provide possibly different features to start modeling from. Using another set of input features can be useful if modeling from a given set of input features seems challenging. Furthermore, the number of features returned by the PFA can be an initial guess for an mRMR method for the size of its selection of features in order to delimitate the combinatorial effort. The basic difference of the PFA and an mRMR method is in deleting all features that are a function of features instead of solving integer optimization problems to find a selection of features optimizing different scores.

Discussion

Next, we discuss the experience that we made with the chi-square test during the experiments for the presented results. In this work a chi-square test was used to identify the independency of two random variables. The binning of random variables, i.e. the discretization of the co-domains of continuous random variables, had an effect on the results and thus the strategy for the binning was crucial. The bin size influences how well the continuous range of a random variable is approximated by the discretized co-domain and thus how well the discretization represents the actual distribution of values of the random variable. On the one hand if the binning of the random variables was too fine, i.e. there were many bins with only a little number of data points each bin, we fell below the recommended threshold for the minimum number of data points in a bin consisting of the cross product of the discretized co-domains of each two random variables for the chi-square test (see the definition of $f_E$ in Section 2 for details about the cross product bin). On the other hand, if the binning of a random variable was too coarse, that means there is only a small number of bins for this variable, the structure of the co-domain of the random variable was lost where e.g. more random variables were sorted as a constant function.

The structure of the co-domain is important for testing the relation of two variables and the capability to predict the output function though. The binning strategy may have an influence on the result. However, since the machine learning models are independent of the binning, the sufficient prediction results on the test data sets of the machine learning models indicate that the approximation of the continuous co-domains via the binning recovered sufficient information. In order to find a good bin size, we recommend the following strategy to find a bin size $\nu$ in Algorithm 4. Start with a small bin size. If the PFA alerts that there is a bin consisting of the cross product of the discretized co-domains of two random variables in the chi-square test with less than the recommended number of data points (default is 5), then slightly increase $\nu$ until there is no alert. By the slight increments of $\nu$ as much of the continuous structure of the co-domain of the continuous random variables as possible can be preserved.

The chi-square test can be so much the better be applied in cases where the co-domain of the random variables is naturally discretized. An example could be in bioinformatics where the expression level of genes is classified in low, medium and high and the cell state is either pathological or physiological.

Conclusion

In this work the PFA was presented. The basic idea of the PFA is to reduce a set of features by identifying features that are functions of other features and sort the functions out such that only these features are left that are the arguments of the functions. If necessary the features that are functions can be modeled from the arguments. The basic ingredients for the PFA is a dependency graph that is built from information about the relation of two features. In the dependency graph functions of features generate special structures that are detected with a minimal cut algorithm. Thus redundancies in the data set can be reduced and the modeling can be focused on the relevant independent input features.

The reduction of data sets improves their processing and opportunities to understand the relations of the underlying processes. In particular, since the reduction of features takes place on the original data set without transforming them into new composite features, the contribution of the PFA will enhance the explainability of machine learning models. Furthermore, mechanistic modeling will be simplified since the PFA can provide candidates to construct input-output-interfaces via which well analyzed submodels can be assembled together to a total model. Moreover, the PFA will contribute to the capability of humans to learn from unsupervised machine learning algorithms by extracting the features whose values are relevant for the clustering of the machine learning model.
The runtime of the PFA can be further developed by improving the minimal cut algorithm provided by the networkx library for dissecting the graph. Furthermore, the provided code can be parallelized in order to process several of the sub graphs in the PFA method at the same time. In addition the provided Python code can be transformed to a hardware near programming language.

Supplementary material

We provide a Python implementation of the presented framework. The three files are:

- execute_relevant_PFA.py
- find_relevant_principle_features.py
- principle_feature_analysis.py

The implementation can be used for any data set with one output function and can be easily extended to be used for more than one output function. In the file execute_relevant_PFA.py, we enter the path of the considered csv-file in which the data is stored as follows. For each data point a column is used where in the first row we have the value of the output function and in the remaining rows there are the values of each feature for the corresponding data point. By executing execute_relevant_PFA.py the left two functions are automatically run and the principle variables are presented as numbers corresponding to the row number of the input csv-file (number 1 is the input function, number 2 corresponds to the first feature, ...).

In the zip-file data_server.zip there is the train and the test file used for the results presented in Table 1 and Table 2 in Section 3. In the zip-file data_single_cell.zip, we have the train and test data to generate the results presented in Section 4.

The script classification.py was used to train the NN and the SVM from the selected features encoded as a list of numbers corresponding to the rows of the corresponding csv-file. The script is provided to simplify the confirmability of the presented results.

The script process_data_for_mRMR.py can be used to transform the csv-file in which the data points are stored for the PFA to a csv-file for the mRMR method from [http://home.penglab.com/proj/mRMR/](http://home.penglab.com/proj/mRMR/). The version that was used in this work is provided in the folder mRMR_c_source_code.

A link where the supplementary material can be downloaded will be available in a version of the presented work published in a journal.

Authors’ contributions

TB developed the PFA and implemented the PFA in Python. TB was mainly involved in writing. LR set up the data center to create the data for Section 3 and was involved in writing. CL researched and preprocessed the data set for Section 4 and was involved in writing. PJ contributed to evaluating the PFA presented in Section 3 and was involved in writing.

Conflicts of interests

The authors declare no conflict of interest.

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Appendix

In the appendix, we give further technical details about how to discretize the co-domain of our random variables in order to transform continuous random variables into discrete random variables, i.e. variables with a finite number
of outcomes. Furthermore, we discuss requirements such that we can apply our framework based on the chi-square test.

Next, we give and subsequently discuss an algorithm to discretize the co-domain of random variables, i.e. bin the values of the random variables. We remark that this procedure works well for our data. However, one can think of different methods that suits a certain scenario to discretize the continuous random variables.

Algorithm 4 Discretize the co-domain of random variables

1. Set $\nu \in \mathbb{N}$ number of minimum number a bin

2. For any random variable $x$
   
   (a) Determine the minimum value $m$ and the maximum value $M$ of all measured values of $x$
   
   (b) If $M \leq m$: Skip $x$
   
   (c) If $M > m$:
      
      i. Sort the measured data points of $x$ in ascending order.
      
      ii. Go through the data points in ascending order. Determine the range of a bin such that there are at least $\nu$ data points within the current bin and that the value of the last data point of the current bin is greater than the first one of the next bin.
      
      iii. If there are less then $\nu$ data points left: Join these data points with the last bin that has at least $\nu$ data points.

Algorithm 4 works as follows. After setting the parameter $\nu$, the following steps are performed for any random variable whose co-domain we would like to discretize. We first determine the minimum and the maximum value of the measure points of $x$. If $M \leq m$, it means that the random variable is constant according to our measurements. In this case, we skip the random variable since we cannot gain information regarding the output function. If $M > m$, then we go through the ordered data points and put the following $\nu$ data points into one bin. If the value of the current data point equals the value of the next data point that is not yet put into a bin, we additionally put all the further data points into the current bin until the value of the next data point is greater than the value of the last data point that is part of the current bin. Then we start to generate a new bin. If there are only less then $\nu$ data points left, which are not put into a bin yet, then we put these data points into the last bin with at least $\nu$ data points. Below, we explain the importance of the parameter $\nu$ and the consequences of its value for the chi-square test.

Next, we discuss the distribution of the random variables $\chi_{ij}$ defined in (3) for any $i \in \{1, \ldots, k\}$ and $j \in \{1, \ldots, l\}$ and their mutual independence. These random variables each are approximately normally distributed with expectation zero and variance one and mutually independent as follows. The discussion will give us some insight into the requirements for our data set such that the presented framework provides reliable results.

In our setting of Section 2, we perform $n_m$ measurements and we count how often two random variables take each a value assigned to a certain bin. We refer to two random variables taking each a value assigned to a certain bin as the considered event. Our model for the measurement is the following. The data points are randomly drawn from a huge amount of measured data points. The probability that the drawn data point has the value within the considered bin is denoted with $p \in (0, 1)$. We assume that the conditions for our experimental setting are constant such that $p$ is a constant for any repetition of a measurement series. Consequently, the number of counts how often our considered event happens within $n_m$ measurements is the expectation of a Bernoulli experiment with the binary Bernoulli variable which models the outcome of a measurement that our considered event happens or not. The number of counts is a random variable denoted with $v$. The probability that we have $m_v$ counts of our considered event within a period of measurement is given by the Binomial distribution

$$P_B (m_v) = \binom{n_m}{m_v} p^{m_v} (1 - p)^{n_m - m_v}. \quad (5)$$

Further, we have the following relation

$$n_m p = \lambda \quad (6)$$

where $\lambda$ is the expectation of counts of our considered event within $n_m$ measurements.

Since in our scenarios we usually have $m_v$, $\lambda$ and not $p$, we use (6) to replace $p$ in (5) by $m_v$ and $\lambda$. We can simplify the Bernoulli distribution since we assume that $n_m$ is large compared to $m_v$. By applying this assumption
that \( n_m \) is large compared to \( m_v \), the Bernoulli distribution can be approximated by the Poisson distribution as follows. We have

\[
\lim_{n_m \to \infty} P_B(m_v) = \lim_{n_m \to \infty} \left( \frac{n_m}{m_v} \right) p^{m_v} (1-p)^{n_m-m_v}
\]

\[
= \lim_{n_m \to \infty} \left( \frac{n_m!}{(n_m-m_v)!m_v!} \right) \left( \frac{\lambda}{n_m} \right)^{m_v} \left( 1 - \frac{\lambda}{n_m} \right)^{n_m-m_v}
\]

\[
= \lim_{n_m \to \infty} \left( \frac{n_m!}{n_m^m (n_m-m_v)!} \right) \left( 1 - \frac{\lambda}{n_m} \right)^{m_v} \left( 1 - \frac{\lambda}{n_m} \right)^{n_m}
\]

\[
= \lim_{n_m \to \infty} \left( \frac{n_m!}{n_m^m (n_m-m_v)!} \right) \left( 1 - \frac{\lambda}{n_m} \right)^{m_v} \left( 1 - \frac{\lambda}{n_m} \right)^{n_m}
\]

\[
= 1 \cdot \frac{\lambda^{m_v}}{m_v!} e^{-\lambda}
\]

where we use the calculation rules for the limit, see [1] II.2 2.2 Proposition, 2.4 Proposition] for example, the definition of the exponential function \( \lim_{n \to \infty} \left( 1 - \frac{x}{n} \right)^n = e^{-x} \), see [1] III.6.23 Theorem] for instance and the definition of the binomial coefficient \( \binom{n_m}{m_v} := \frac{n_m!}{(n_m-m_v)! m_v!} \). As expected the Poisson distribution has expectation and variance \( \lambda \), see [1] Example 1.6.4 or [33] 1.3.4 Poisson distribution] for example.

Now, we show that the Poisson distribution can be approximated by a normal distribution for \( \lambda \) sufficiently large and thus that \( \chi_{ij} \) for any \( i \in \{1, \ldots, k\} \) and \( j \in \{1, \ldots, l\} \) is normally distributed for \( \lambda \) sufficiently large. Since the conditions in our scenario are assumed to be constant and the data points are randomly drawn, the following two ways to measure the counts of our considered event are supposed to be equivalent. We can measure the counts of our considered event drawing \( n_m \) data points at once. Equivalently, we can divide the \( n_m \) measurements into several smaller sub measurement series such that the sum of all measurements equals \( n_m \) as well and then sum up all the sub expectations from any sub measurement series to obtain the expectation of the total measurement where we perform the measurement in one part. According to the assumption that the data points are drawn randomly, the counts of our considered event in any sub measurement series are mutually independent random variables following each a Poisson distribution with corresponding expectation and variance. The corresponding mutually independent random variables in each sub measurement series are denoted with \( \chi_{i,j} \), \( i \in \{1, \ldots, n_v\} \) where \( n_v \in \mathbb{N} \) is the number of sub measurement series of the total measurement series. Consequently, we can model the process of measuring the counts of our considered event with the random variable \( S = \sum_{i=1}^{n_v} \chi_{i,j} \) for the total measurement series.

Next, we show that \( S \) is also Poisson distributed where the expectation is the sum of all the expectations of the Poisson distributions for the sub measurements \( \chi_{i,j} \). Analogously, for the variance. We show the Poisson distribution of \( S \) by iteratively merging two Poisson distributions. Since \( v_i \) are mutually independent, the probability that the sum of \( v_i \) and \( v_j, i \neq j \), equals \( N_v \in \mathbb{N} \cup \{0\} \) is given by

\[
P \left( v_i + v_j = N_v \right) = \sum_{m_{v_i}=0}^{N_v} P_{v_i}(m_{v_i}) \cdot P_{v_j}(N_v - m_{v_i})
\]

where \( P_{v_i}, v \in \{v_i, v_j\} \) is the corresponding Poisson distribution for \( v_i \), resp., \( v_j \) with corresponding expectation and variance. By the virtue of the Binomial theorem, see [1] I.8.4 Theorem] for example, we have, analogously to [20], that the distribution of the sum of \( v_i \) and \( v_j \) is also Poisson distributed with an expectation being equal to the sum of the expectation of \( P_{v_i} \) and \( P_{v_j} \). The same holds for the variance.

Due to the reasoning of the last paragraph, we can consider a series of measurements where our considered event occurred \( \lambda \) times as a Poisson distributed random variable decomposed of \( \lambda \) random variables that are Poisson distributed with each expectation one. For example we can choose the length of the sub measurement series sufficiently small such that the expected occurrence of our considered event on this sub interval equals one.

Now, we switch to Section 2 to see that \( \chi_{ij} \) for any \( i \in \{1, \ldots, k\} \) and \( j \in \{1, \ldots, l\} \) is normally distributed for \( \lambda \) sufficiently large and mutually independent for all \( i \in \{1, \ldots, k\} \) and \( j \in \{1, \ldots, l\} \). We have that the counts where our considered event happens, named by \( f_0(i,j) \) for each \( i \in \{1, \ldots, k\} \) and \( j \in \{1, \ldots, l\} \), is considered as a sum of \( f_E(i,j) \) (which has the role of \( \lambda \) in the discussion above) Poisson distributed mutually independent random variables each with expectation one and variance one. Consequently, we apply the Central Limit Theorem, see [20] Theorem 15.37, to obtain that \( \chi_{ij} \) for each \( i \in \{1, \ldots, k\} \) and \( j \in \{1, \ldots, l\} \) is (approximately) normally distributed
as follows. If $f_E(i,j)$ is sufficiently large, we have that $\chi_{ij}$ is normally distributed with expectation zero and variance one for each $i \in \{1,\ldots,k\}$ and $j \in \{1,\ldots,l\}$. Next, we consider the mutual independence of the $\chi_{ij}$ for all $i \in \{1,\ldots,k\}$ and $j \in \{1,\ldots,l\}$. Analogously to the reasoning above for the random variable $v$ describing that a data point is in a certain bin, we can define such a random variable for any bin to which the values of the considered two random variables are assigned to. Repeating the measurement series several times under constant conditions, the variable $f_O(i,j)$ is the random variable modeling the counts that the value of a data point is assigned to the bin parametrized with $i \in \{1,\ldots,k\}$ and $j \in \{1,\ldots,l\}$. Since the data points are randomly drawn from the huge amount of data points with constant experimental settings, the expectation and variance $f_E(i,j)$ is assumed constant in any sweep of a measurement series for any $i \in \{1,\ldots,k\}$ and $j \in \{1,\ldots,l\}$. As a consequence the random variables $\chi_{ij}$ are mutually independent for all $i \in \{1,\ldots,k\}$ and $j \in \{1,\ldots,l\}$.

According to the reasoning of the last paragraph, we can apply the chi-square test to $\chi^2$ defined in [2] as follows. Since the random variables $\chi_{ij}$ are mutually independent and (approximately) normally distributed, the random variable $\chi^2$ is chi-square distributed as a sum of normally distributed independent random variables, see [8, Chapter 18] for example. From the chi-square distribution, the probability to obtain a $\chi^2$ value greater or equal than the given value of $\chi^2$ can be calculated. A probability for obtaining $\chi^2$ values greater or equal than the given value of $\chi^2$ of the performed measurement series below a predefined threshold (level of significance) indicates that the obtained $\chi^2$ values, resulting from the deviations of $f_O(i,j)$ and $f_E(i,j)$ for one $i \in \{1,\ldots,k\}$ and $j \in \{1,\ldots,l\}$, is unlikely. Although all the assumptions are fulfilled, in particular that the considered random variables are independent, an unlikely outcome of a random experiment can be coincidence and thus possible. In our case however, if the probability to obtain a $\chi^2$ value greater or equal than the given value of $\chi^2$ is below a predefined threshold, we assume that one assumption must be violated. Since the conditions during our experiments can be assumed constant and the data points are randomly drawn, we assume that most likely $\chi_{ij}$ is not normally distributed with zero expectation for one $i \in \{1,\ldots,k\}$ and $j \in \{1,\ldots,l\}$. Consequently, $f_E(i,j)$ is not the expectation of $f_O(i,j)$ for one $i \in \{1,\ldots,k\}$ and $j \in \{1,\ldots,l\}$ meaning we reject the hypothesis that the corresponding random variables are independent since (1) is not fulfilled for all $i \in \{1,\ldots,k\}$ and $j \in \{1,\ldots,l\}$ within our statistical tolerances.

Remark 13. We remark that in literature it is a common recommendation to have five data points in a bin [27], i.e. $f_O(i,j) \geq 5$ for each $i \in \{1,\ldots,k\}$ and $j \in \{1,\ldots,l\}$, to consider $f_E$ as sufficiently large such that the corresponding Poisson distribution is approximately a normal distribution. By increasing the parameter $\nu$ in Algorithm 4, we can increase the number of data points in a bin, i.e. $f_E(i,j)$ is increased for each $i \in \{1,\ldots,k\}$ and $j \in \{1,\ldots,l\}$, until the condition that $f_E(i,j) \geq 5$ for each $i \in \{1,\ldots,k\}$ and $j \in \{1,\ldots,l\}$ is fulfilled or any other desired lower bound for $f_E(i,j)$.

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