Abstract
Principal Component Analysis (PCA) is a well known procedure to reduce intrinsic complexity of a dataset, essentially through simplifying the covariance structure or the correlation structure. We introduce a novel algebraic, model-based point of view and provide in particular an extension of the PCA to distributions without second moments by formulating the PCA as a best low rank approximation problem. In contrast to hitherto existing approaches, the approximation is based on a kind of spectral representation, and not on the real space. Nonetheless, the prominent role of the eigenvectors is here reduced to define the approximating surface and its maximal dimension. In this perspective, our approach is close to the original idea of Pearson [1901] and hence to autoencoders. Since variable selection in linear regression can be seen as a special case of our extension, our approach gives some insight, why the various variable selection methods, such as forward selection and best subset selection, cannot be expected to coincide. The linear regression model itself and the PCA regression appear as limit cases.

Keywords: $\alpha$-stable, extreme values, monoids, matrix-valued, PCA, PCA regression

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1 Introduction
Principal Component Analysis (PCA), introduced by Pearson [1901], has been one of the most commonly used statistical methods for reducing the complexity in datasets: for $n$ samples with a high number of features $p$, a linear subspace is chosen in favor of a simpler representation of the data. Under the assumption of existing variances, these applications have been justified by many theoretical results and have been applied successfully in a wide variety of scientific fields. Overviews can be found in [Hastie, 2009, Jolliffe, 2002, Ringnér, 2008], for instance. Some special care is needed when the distribution of the data deviates considerably from the multivariate normal distribution.
In particular, probability laws without second moments or counting distributions may lack theoretical justification or a good interpretation when PCA is applied (Jolliffe, 2002). Several generalizations have been considered (Bengio et al., 2013; Candès et al., 2011; Hofmann et al., 2008; Silverman, 1990; Vidal et al., 2016). A particularly flexible one is the autoencoder, a neural network architecture that has been considered both in mathematics and statistical learning (Baldi and Hornik, 1989; Jolliffe, 2002; Oja and Karhunen, 1985). The autoencoder is based on the formulation of a regression problem, where the data is reconstructed by a map that simplifies the structure in some sense. Often, simplification is meant in terms of mapping into a lower dimensional space and then back to the original space of the data. Here, the admissible maps are possibly nonlinear and chosen such that a certain loss function is minimized. Classic PCA appears as a special case of choosing linear maps.

Algebra plays a dominant role in founding certain areas of probability theory, in particular stochastic processes (Sasvári, 2005; Schilling et al., 2012; Strokorb and Schlather, 2015). When special problems are addressed, modern algebra has also found applications in statistics, for instance, in design of experiments (Bailey, 2004) or in learning theory (Watanabe, 2009). Surprisingly, when data themselves are considered, ‘linearity’ usually refers to vector spaces over the field of real numbers, although many random variables exhibit natural linearity with respect to other operations (Golan, 1999; P. Prakash, 1974). An exception in extreme value theory is Gissibl et al. (2021) who refer to the tropical algebra, however in a different context than PCA. Distributions with a stability to some given algebraic operation typically stem from limit laws and hence are infinitely divisible, again not necessarily with respect to the field of real numbers (Davydov et al., 2008). In our algebraic approach, the classic PCA reappears as the Gaussian case.

A particular class of distributions without guaranteed second moments, which exhibits linearity with respect to maxima instead of addition, are the max-stable distributions (L. de Haan, 2006; Resnick, 1987; Stoev and Taqqu, 2003). In contrast to the multivariate Gaussian distribution, the dependence structure of max-stable distributions cannot be fully described by bivariate characteristics like the covariance (Beirlant et al., 2004; Strokorb and Schlather, 2015). Hence, decomposing any such derived matrix cannot be sufficient, at least from a theoretical point of view (Jiang et al., 2020).

We consider here also intrinsically vector-valued data, which appear in colour coding, for instance. Special cases there of are matrix-valued data, which appear in a single measurement, for example in functional magnetic resonance imaging (Wang et al., 2016). Linear regression models can also be seen as a special case of vector-valued data. Both variable selection and classic PCA are dimension reducing methods. The ideas are frequently combined, leading to the PCA regression analysis or the sparse PCA, for instance (Hastie, 2009). Nonetheless, variable selection and PCA have been considered as different methods.

Central part of the paper is the definition of the generalized PCA in Section 3. It is based on generalizations of several well-known notions, such as stable distributions and quadratic variation (Section 2). An important specification of our approach is the PCA for extreme values (Section 4). Some background information is given in the appendix.
2 Foundations

Since classic PCA minimizes the mean square of the residuals (Pearson, 1901), calculating the difference between random variables is implicitly required. In our generalization towards extreme values with Fréchet margins, we replace the abelian group \((\mathbb{R}, +)\) by the semi-group \(([0, \infty), \vee)\) where \(a \vee b := \max\{a, b\}\). Since the calculation of a difference is impossible in a semi-group context, we provide a workaround for the mean square of the residuals, here. First, we have to declare for which random vectors we have a workaround (Section 2.3). Essentially, these vectors have a stable distribution (Section 2.2). In Subsection 2.6 we define a convenient distance between random vectors, which avoids the calculation of residuals. This semi-metric is based on a semi-scalar product (Subsection 2.5), which itself is based on a kind of valuation principle (Subsection 2.4). The latter is fundamental, since it (i) generalizes the quadratic variation, (ii) is unique in important cases and (iii) throws new light on the variance.

2.1 Semigroups and Semirings

Since semigroups are not that frequently used in a statistical context, we repeat basic notions. See Golan (1999) for a general introduction, for instance. Throughout the paper, we will use +, \(\vee\), +, and \(\tilde{+}\) for the binary operator of the standard addition, the maximum, a general semigroups and a general semiring, respectively. The corresponding multi-operators are denoted by \(\sum\), \(\bigvee\), \(\sum\) and \(\tilde{\sum}\).

Definition 2.1. Let \(G\) be a nonempty set and \(+: G \times G \rightarrow G\) be an associative operation, then the tuple \((G, +)\) is called a semigroup. A semigroup is called

1. a monoid with identity element 0, if an element \(0 \in G\) exists, such that \(\alpha + 0 = 0 + \alpha = \alpha\) for all \(\alpha \in G\).
2. commutative, if \(\alpha_1 + \alpha_2 = \alpha_2 + \alpha_1\) for all \(\alpha_1, \alpha_2 \in G\).
3. topological, if the set \(G\) has a topology \(\tau\), \((G, \tau)\) is a topological space and the map \(+: G \times G \rightarrow G, (\alpha_1, \alpha_2) \mapsto \alpha_1 + \alpha_2\) is continuous.

Definition 2.2. A set \((R, \tilde{+}, \cdot)\) with addition \(\tilde{+}\) and multiplication \(\cdot\) is called a semiring if

1. \((R, \tilde{+})\) is a commutative monoid with identity element 0,
2. \((R, \cdot)\) is a monoid with identity element 1,
3. multiplication is left and right distributive, i.e., \(\alpha_1(\alpha_2 \tilde{+} \alpha_3) = \alpha_1 \alpha_2 \tilde{+} \alpha_1 \alpha_3\) and \((\alpha_2 \tilde{+} \alpha_3)\alpha_1 = \alpha_2 \alpha_1 \tilde{+} \alpha_3 \alpha_1\)
4. \(0 \cdot \alpha = \alpha \cdot 0 = 0\) for all \(\alpha \in R\).
Example 2.3. Examples of practically relevant semirings are, for instance, \((X, +, \cdot)\) with \(X \in \{\mathbb{R}, \mathbb{Z}, \mathbb{N}_0, [0, \infty)\}, ((0, \infty), \vee, \cdot), (\mathbb{R}, \vee, +)\), and \((\mathbb{R}^{d \times d}, +, *)\), where \(*\) denotes the matrix multiplication. If \(M\) is a non-empty set, then \((2^M, \cup, \cap)\) is also a semiring. Last but not least, the quaternion number system is a semiring, which is used in certain areas of physics, see [Menanno and Mazzotti (2012)], for instance.

Essentially, the definition of a semiring means that the inverses with respect to addition and multiplication are missing and that the multiplication is not necessarily commutative. However, we will always assume that + is commutative, \(G\) and \(R\) have at least two elements, and that \(G\) and \(R\) are topological. Since the focus of the paper is on algebraic aspects, we assume for ease that both, \(G\) and \(R\), are Polish. Furthermore, we will drop the multiplication sign in formulae whenever possible. On the other hand, especially when several different semigroups or semirings are involved in a formula, we may clarify neutral elements and operators with indices.

In our set-up, the “scalar” random variable takes values in a monoid \(G\). Much more structure will be imposed on the set \(R\), which indexes the distributions and which will be a semiring. Primarily, it is this index set \(R\) that is extended to higher dimensions, the so-called semimodule.

Definition 2.4. Let \((S, \oplus)\) be a commutative semigroup and \((R, \hat{+}, \cdot)\) a semiring. Let \(\odot: R \times S \to S\) be a mapping that satisfies for all \(\alpha, \beta \in R\) and \(x, y \in S\) the following properties:

\[
\begin{align*}
\alpha \odot (\beta \odot x) &= (\alpha \beta) \odot x \\
\alpha \odot (x \oplus y) &= (\alpha \odot x) \oplus (\alpha \odot y) \\
(\alpha \hat{+} \beta) \odot x &= (\alpha \odot x) \oplus (\beta \odot x) \\
1_R \odot x &= x, \ 0_R \odot x = x \odot 0_S = 0_S.
\end{align*}
\]

Then \(S\) is called a semimodule over \(R\). A subset \(V \subset S\) that obeys the above conditions is called a subsemimodule. If \((S, \oplus)\) is a topological semigroup and \(\odot\) is continuous, the semimodule is called topological. We write \((S, \hat{+})\) and \(\cdot\) instead of \(\odot\), if \(S\) is canonic, e.g., if \(S = \mathbb{R}^d\) for some \(d \in \mathbb{N}\).

Definition 2.5. Let \(S\) be a semimodule and \(B \subset S\). Let \(#B\) be the cardinality of \(B\). The value

\[
\text{rank } S := \min \{#B : S = \text{span } (B)\}
\]

is called the rank of \(S\).

Note that the span in the preceding definition is calculated according to the semimodule operations. Linear maps will play an essential role for the reconstruction of the points.

Definition 2.6. Let \(S_1\) and \(S_2\) be topological semimodules over the same semiring \((R, \hat{+}, \cdot)\), with the commutative semigroups \((S_1, \oplus_{S_1})\) and \((S_2, \oplus_{S_2})\). A map \(H: S_1 \to S_2\) satisfying the conditions

\[
H(\lambda x) = \lambda H(x) \quad \forall \lambda \in R, x \in S_1
\]
\[ H(x \oplus S_1 y) = H(x) \oplus S_2 H(y) \quad \forall x, y \in S_1 \]

is called \( \oplus S_1 - \oplus S_2 - \text{linear} \). If \( S_1 \) and \( S_2 \) are both canonical, then \( H \) is called \( \overset{\text{+}}{\text{-linear}} \).

**Remark 2.7.** If \( S_1 = R^d \) and \( S_2 = R^p \), a \( \overset{\text{+}}{\text{-linear}} \) map \( H \) can always be represented by a matrix \( H \in R^{p \times d} \) such that

\[ Hx := \left( \sum_{j=1}^{d} H_{ij}x_j \right)_{i=1,\ldots,p}, \quad x \in \mathbb{R}^d. \]

Although the definitions above are in analogy to the definitions of a vector space and a linear mapping, the consequences of the transition from groups to semi-groups are severe. For instance, the dimension of a subspace of a finite dimensional space does not necessarily exist. Appendix A gives some implications that are particularly important when dealing with extreme values. Appendix A also delivers implicitly arguments, why a constructive approach via explicit multivariate distributions is chosen to define the generalized PCA, and not via an abstract formulation based on subsemimodules or on the rank of a matrix.

### 2.2 Stable distributions

For a general approach to PCA without existing variance we need a generalized notion of stable distributions, where we replace the standard addition by an arbitrary semigroup operation. Some additional care is needed with respect to the scaling properties of random variables. The following definitions provide the structure to develop a useful theory.

**Definition 2.8.** Let \( (G, \ast) \) be a topological monoid and \( (R, \ast, \cdot) \) a semiring with an additional binary operation \( \circ : R \times R \rightarrow R \). Let \( \mathcal{F} := \{ F_\mu : \mu \in R \} \) be a set of distributions over \( G \) and \( H_\mu : G \rightarrow G, \mu \in R \), measurable maps, such that

\begin{align*}
H_1 &= \text{id}_G \\
H_0 &= 0_G \\
H_\mu(X_\nu) &\sim F_{\mu \nu}, \quad \mu, \nu \in R, X_\nu \sim F_\nu \\
X_\mu + X_\nu &\sim F_{\mu \circ \nu}, \quad X_\mu \sim F_\mu, X_\nu \sim F_\nu \quad \text{independent.}
\end{align*}

(1) \hspace{1cm} (2)

Then, the set \( \mathcal{F} \) is called a *stable set of distributions*. We write briefly \( \mu X_\nu \) instead of \( H_\mu(X_\nu) \).

The following definition ensures that transformations of random vectors have still the required distribution, see Proposition 2.15 below.

**Definition 2.9.** Let \( \mathcal{F} \) be stable set of distributions where all \( H_\mu, \mu \in R \), are linear, then \( \mathcal{F} \) is called *linear.*
Example 2.10. In case of symmetric $\alpha$--stable distributions $S_\alpha(\sigma,0,0)$, $\alpha \in (0,2]$, we have for $\sigma,\tau,\mu \in \mathbb{R}$ that
\[
G \equiv R = \mathbb{R} \\
H_\sigma(x) = \sigma x \\
\sigma \circ \tau = (\sigma^\alpha + \tau^\alpha)^{1/\alpha}.
\]
Hence, the set of symmetric $\alpha$--stable distributions is stable and linear. Here, the Gaussian case is included as $S_2(\sigma,0,0) = \mathcal{N}(0,2\sigma^2)$, see Samorodnitsky and Taqqu (1994).

Example 2.11. Matrix-valued data can be considered as vector-valued with special constraints, which are modelled as a subsemiring of the semiring of matrices. An example of such a subsemiring is a set of block diagonal matrices with fixed block structure. Let us consider here vector-valued data with values in $\mathbb{R}^k$, $k \in \mathbb{N}$. Let
\[
(G, +) = (\mathbb{R}^k, +) \\
(R, +, \cdot) = (\mathbb{R}^{k \times k}, +, \cdot),
\]
where $\cdot$ is the standard matrix multiplication. Then $G$ is an abelian group and $R$ is a non-commutative ring. We identify $R$ with the set of $+$-linear maps, i.e.
\[
H_A : \mathbb{R}^k \to \mathbb{R}^k, x \mapsto Ax \quad \text{for } A \in R,
\]
so that $1_R$ is the identity matrix, for instance. The $F_A, A \in R$, are not distinct, since for any $A, B \in R$ we have
\[
AX_1 \sim BX_1 \iff AA^\top = BB^\top.
\]
Finally, denote by $M^{1/2}$ a (through some alphabetic ordering uniquely defined) square root of a positive semidefinite matrix $M$. Then, for $A, B, C \in R$ and two independent random matrices $X_1, X_1^\top \sim F_1$ we have
\[
A \circ B = (AA^\top + BB^\top)^{1/2}.
\]
Thus, the set of $k$-variate Gaussian distributions is stable and linear.

Example 2.12. Let $(R, +, \cdot) = (\mathbb{R}^{k \times k}, +, \cdot)$ for some $k \geq 1$ as in the previous example. We switch to the standard notation. Let $P \subset R$ be the subsemiring of $k \times k$ matrices $A$ of the form
\[
A = \begin{pmatrix}
A_\sigma & A_\beta \\
0_{(k-1)\times 1} & A_\mu 1_{(k-1)\times (k-1)}
\end{pmatrix},
\]
where $A_\sigma \geq 0$, $A_\mu \geq 0$, $A_\beta \in \mathbb{R}^{1 \times (k-1)}$, $1_{(k-1)\times (k-1)}$ denotes the unity matrix, and $A_\mu = 0$ shall imply $A_\sigma = 0$ and $A_\beta = 0$. Let for $\ell = 1, \ldots, k$
\[
S_\ell := \{A \in P: A_{\beta,j} = 0, j \neq \ell\}, \\
L_\ell := \text{span}(S_1, \ldots, S_\ell) = \{A \in P: A_{\beta,j} = 0 \text{ for } j > \ell\}.
\]
Then, for \( \ell = 1, \ldots, k \), the sets \( S_\ell \) and \( L_\ell \) are subsemirings of \( P \). We interpret this set-up as a framework for linear regression models. Let \( X_1, \ldots, X_{k-1} \) be the predictor variables which are typically assumed to be independent of the error \( \varepsilon \). Since we aim to show later on, that variable selection in linear modelling is a special case of our PCA, we assume that \( Z = (\varepsilon, X_1, \ldots, X_{k-1}) \) has any multivariate Gaussian distribution. Let \( A \in L_k \). Then, \( A_\sigma \) equals the standard deviation of the error if \( \varepsilon \sim \mathcal{N}(0,1) \). The first component of \( AZ \) equals the dependent variable \( y \), i.e.,

\[
y = (AZ)_{11} = \sum_{i=1}^{k-1} A_{\beta,i} X_i + A_\sigma \varepsilon.
\]  

The set \( S_\ell \) corresponds to a simple linear regression model based on \( X_\ell, \ell \geq 2 \). The set \( L_\ell, \ell < k \), denotes the models, where only the predictor variables \( X_i, 1 \leq i \leq \ell \), are considered. In our example, the intercept, which is crucial in practice, is missing, for ease of theoretical reasoning. The family of distributions \( \mathcal{F} \) corresponding to the \( AZ, A \in L_k \), is a stable set, if \( Z \) consists of independent Gaussian components. I.e., it can be shown that one of the roots \( (AA^T + BB^T)^{1/2} \) is in \( L_k \) if \( A \) and \( B \) are. Unfortunately, this is a trivial case for variable selection. For a general distribution of \( Z \), a representation of the linear model as a stable family is unknown. Fortunately, \( R \) itself is rich enough so that the PCA can be applied, cf. Example 3.5.

**Definition 2.13.** Let \( \mathcal{F} \) be a linear, stable set of distributions. If \( 1 \in R \) allows the division by \( n \) in the sense that

\[
\bigotimes_{i=1,\ldots,n} \nu_n = \nu_n \circ \ldots \circ \nu_n = 1
\]

for some \( \nu_n \in R \) and any \( n \in \mathbb{N} \), then \( \mathcal{F} \) is called a set of **infinitely divisible distributions**.

### 2.3 Multivariate distributions

Stable sets of multivariate distributions are already covered by Definition 2.8. Here, we consider an alternative, constructive definition for a multivariate version of a stable distribution that is tailored for our generalized PCA and avoids existence problems. Recall that \( \mu X_\nu \) is an abbreviation for \( H_\mu(X_\nu) \).

**Definition 2.14.** Let \( \mathcal{F} \) a stable set of univariate distributions and \( d, n \in \mathbb{N} \). Let \( \mathcal{F}_{0} \) be the set of distributions given by

\[
\nu W := \sum_{j=1,\ldots,n} \langle \nu_{1j}, \ldots, \nu_{dj} \rangle^T W_j := \sum_{j=1,\ldots,n} \langle \nu_{1j} W_j, \ldots, \nu_{dj} W_j \rangle^T
\]

for all

\[
\nu = (\nu_{ij})_{i=1,\ldots,d; j=1,\ldots,n} \in \mathbb{R}^{d \times n},
\]

independent random variables \( W_j \sim F_{\mu_j}, \mu_j \in R, \) and \( W := (W_1, \ldots, W_n)^T \). We write

\[
\nu W \sim F_{\nu,\mu}^{d}
\]
with \( \mu = (\mu_1, \ldots, \mu_n) \). Let \( \mathcal{F}^d \) be the weak closure of \( \mathcal{F}_0^d \). Then, an element of \( \mathcal{F}^d \) is called a \( d \)-variate \( \mathcal{F} \)-distribution.

We call \((G, R, \mathcal{F}^d)\) a multivariate model. It is called linear if \( \mathcal{F} \) is linear.

Definition 2.14 ensures that the univariate margins of \( F \in \mathcal{F}_0^d \) are in \( \mathcal{F} \). A linear multivariate model ensures that the \( p \)-variate margins of \( F \in \mathcal{F}_0^d \) are in \( \mathcal{F}_0^p \).

**Proposition 2.15.** Let \((G, R, \mathcal{F}_0^d)\) be a linear multivariate model, \( X = (X_1, \ldots, X_d) \sim F_{\nu,\mu}^d \), \( \xi = (\xi_1, \ldots, \xi_p) \in R^{p \times d} \), and

\[
\xi X := (\xi_k X)_{k=1}^{p} \quad \text{with} \quad \xi_k X = \sum_{i=1}^{d} \xi_{ki} X_i.
\]

Then

\[
\xi X \sim F_{\xi \nu,\mu}^d.
\]

**Proof.**

\[
\xi_k X = \sum_{i=1}^{d} \xi_{ki} \left( \sum_{j=1}^{n} \nu_{ij} W_j \right) = \sum_{i=1}^{d} \sum_{j=1}^{n} \xi_{ki} \nu_{ij} W_j = \sum_{j=1}^{n} \left( \sum_{i=1}^{d} \xi_{ki} \nu_{ij} \right) W_j.
\]

**Remark 2.16.** Both Definition 2.8 and Definition 2.14 can be generalized slightly, replacing \( H_\mu \) by \( H_{\nu,\mu} \), which is then applied to random vectors \( X_\nu \sim F_\nu \), only. Then, Equation (4) is rewritten as

\[
X = \sum_{j=1}^{n} \left( H_{\nu_1,\mu_1} \cdots H_{\nu_d,\mu_d} \right)^T W_j := \left( \sum_{j=1}^{n} H_{\nu_1,\mu_1} W_j \right)_{i=1}^{d}.
\]

Assume \( G \subset \mathbb{R} \) and all \( F \in \mathcal{F} \) are continuous and distinct, i.e., \( F_\mu \neq F_\nu \) for \( \nu \neq \mu \). Then \( H_{\nu,\mu} = F_\nu^{-1}(F_\mu(x)) \) is a possible choice. Here, \( F_\nu^{-1} \) denotes the pseudoinverse of \( F_\nu \). In practice, monotonously increasing maps \( H_{\nu,\mu} \) are preferred so that the \( H_{\nu,\mu} \) are essentially unique. Hence, the generalized map \( H_{\nu,\mu} \) suggests that our approach so far is essentially restricted to continuous distributions.

The set of Gamma distributions \( F_\mu \) with fixed scale parameter and arbitrary non-negative shape parameters \( \mu \geq 0 \) obeys this generalized framework, but fails to be a stable set.

### 2.4 Variation

In classic PCA the mean square of the residuals is minimized. From a model-based perspective, this refers to minimizing the variance of the residuals. In our general approach, the existence of the variance is not guaranteed, so that we have to consider a general function that attaches value to a residual. We wish to minimize the sum of these attached values, but face the additional difficulty that the calculation of the residuals would need additive inverses.

We call the function that attaches values to a random variable a variation, in generalization to the quadratic variation of a Wiener process. Due to property (9) below, it might be interpreted as the number of underlying independent variables.
Definition 2.17. Let $\mathcal{F}$ be a stable set of distributions. A continuous map $[\cdot] : R \to [0, \infty]$ is called a variation, if the following conditions hold

$$
[\mu] = [\nu], \quad \text{if } F_\mu = F_\nu \quad \text{(consistent)} (6)
$$
$$
[\mu] > 0, \quad \mu \in R \setminus \{0\} \quad \text{(positive)} (7)
$$
$$
[0] = 0 \quad \text{(degenerate element)} (8)
$$
$$
[\mu \circ \nu] = [\mu] + [\nu], \quad \mu, \nu \in R \quad \text{(additive)} (9)
$$

We call a variation scale invariant if, additionally,

$$
[\mu \nu] = [\mu] [\nu] \quad \text{for all } \mu, \nu \in R. \quad (10)
$$

We also write $[X]$ and $[F]$ for $X \sim F$ and $F \in \mathcal{F}$.

Remark 2.18. 1. If $[\cdot]$ is scale invariant, we have $[\mu X_\nu] = [\mu] [X_\nu]$, so that rescaling of all components with the same value will not change the outcome of a PCA, provided the sets $B$ and $I$ in Definition 3.2 are also scale invariant.

2. The function $(\mu, \nu) \mapsto [\mu \circ \nu]$ is negative definite, as is any function of the form $(x, y) \mapsto f(x) + f(y)$. Furthermore, $e^{[\cdot]}$ is a semi-character on $(R, \circ)$ with the identity as involution (Berg et al., 1984).

Proposition 2.19. If $[\cdot]$ is scale invariant, then the following properties hold:

1. $[1_R] = 1 \in \mathbb{R}$ for the neutral element $1_R$ of $(R, \cdot)$.
2. $R$ is division free, i.e., for all $\alpha_1, \alpha_2 \in R$ with $\alpha_1 \cdot \alpha_2 = 0$ we have $\alpha_1 = 0$ or $\alpha_2 = 0$.
3. Let $(R, \cdot) \subset (\mathbb{R}, \cdot)$ be a non-trivial interval with standard topology. Then, $[\mu] = |\mu|^{\alpha}$ for some unique $\alpha \in \mathbb{R} \setminus \{0\}$.

Proof.

1. Equality (10) yields $[1_R] = [1_R]^2$. The positivity of the variation excludes $[1_R] = 0$. Hence, $[1_R] = 1$.

2. $0 = [\mu \nu] = [\mu] [\nu]$ implies that $[\mu] = 0$ or $[\nu] = 0$. The positivity of the variation yields $\mu = 0$ or $\nu = 0$.

3. Let $A = \{\log(x) : x \in R \cap (0, \infty)\}$. The function $\ell : A \to \mathbb{R}$, $x \mapsto \log [e^x]$ is well defined on some nontrivial interval that includes 0 and is continuous there. Since $\ell$ obeys Cauchy’s functional equation we get $[\mu] = \mu^{\alpha}$ for $\mu \in R \cap (0, \infty)$ and some $\alpha \in \mathbb{R}$. Now, assume that $R \cap (-\infty, 0) \neq \emptyset$. Then, Cauchy’s functional equation delivers that $[\mu] = |\mu|^{\beta}$ for $\mu \in R \cap (-\infty, 0)$ and some $\beta \in \mathbb{R}$. For $\mu \in R \cap [-1, 0)$ we have $|\mu|, \mu^2 \in R$, so that $[\mu]^2 = [\mu^2] = [\mu^2] = [\mu]^{2}$. Hence $\alpha = \beta$. The additivity yields $|\mu \circ \nu|^{\alpha} = |\mu|^{\alpha} + |\nu|^{\alpha}$ with $\alpha \neq 0$. Assume $\alpha = 0$. Then the continuity of the variation yields $1 = [1 \circ 1] = 1^0 + 1^0$ in contradiction to (9). Now,
assume that $\| \cdot \|_\alpha : \mu \mapsto \mu^\alpha$ and $\| \cdot \|_\beta : \mu \mapsto \mu^\beta$ are two scale invariant variations with $\alpha, \beta \in \mathbb{R}\setminus\{0\}$. Then, for all $\mu \in R$,
\[
(1 + |\mu|^\alpha)^{1/\alpha} = |1_R \circ \mu| = (1 + |\mu|^\beta)^{1/\beta},
\]
so that $\alpha = \beta$.

Example 2.20. In the symmetric $\alpha$-stable case, the so-called covariation norm $\| \cdot \|$ assigns the parameter $\sigma \in R := [0, \infty)$ to $X \sim S_\alpha(\sigma, 0, 0)$ for $\alpha \in (1, 2]$, i.e., $\|X\|_\alpha = \sigma$. It follows immediately from the properties of $S_\alpha(\sigma, 0, 0)$, see Samorodnitsky and Taqqu (1994), that $\|X\|_\alpha^\alpha$ satisfies the four properties of a scale invariant variation, that is, $[\sigma] = \|X\|_\alpha^\alpha$. For centered Gaussian variables with $F_1 = \mathcal{N}(0,1)$, the variation equals indeed the variance.

Example 2.21. In case of the the stable set of $k$-variate Gaussian distributions, see Example 2.11 the variation might be defined as
\[
\| A \| := \text{tr}(AA^\top) = \sum_{i=1}^{k} \sum_{j=1}^{k} A_{ij}^2, \quad A \in R := \mathbb{R}^{k \times k}.
\]

Then, $R$ is division free if and only if $k = 1$.

2.5 Semi-scalar product

Property (9) of the variation gives reason to generalize the notion “uncorrelated” to random variables without existing variance. The following definition is tailor-made for scale-invariant variations.

Definition 2.22. Let $(G, R, \mathcal{F})$ be a multivariate model, $\| \cdot \|$ a variation and $\| 1 + 1 \| = 2$. Let $X$ and $Y$ be random vectors such that their distribution and that of $X + Y$ are in $\mathcal{F}$. For $\mu \in R^d$ let $[\mu]$ be an extension of the variation to a vector $\mu$. Then,
\[
\langle X, Y \rangle := \frac{[X + Y] - [X] - [Y]}{[1+1] - 2}
\]
is called the semi-scalar product between $X$ and $Y$. The vectors $X$ and $Y$ are called uncorrelated (positively / negatively correlated) if $\langle X, Y \rangle = 0$ ($\geq 0$ respectively $\leq 0$).

Remark 2.23. Given the definition of a variation in the univariate case, the definition of the variation of a vector is not clear cut. A convenient definition is
\[
[\mu] := \sum_{i=1}^{d} [\mu_i],
\]
as it ensures (6)–(9) without further assumptions.
Example 2.24. Let $X$ be a standard Gaussian random variable and the variation of a vector be the sum of the variation of the components. Then the random vectors $(1, -1)^T X$ and $(1, 1)^T X$ are jointly multivariate Gaussian, fully dependent, but uncorrelated according to Definition 2.22. Note that the standard notion of “uncorrelated” is defined only for scalar random variables. The generalized definition still implies that two jointly bivariate, scalar Gaussian random variables are uncorrelated if and only if they are independent.

Example 2.25. In the max-stable case the operator $\max$ is the maximum, so that $1 \max 1 = 1$ and hence $[1+1] - 2 = -1 \neq 0$. In the case of $\alpha$-stable distributions, however, the case $\alpha = 1$ leads to $[1+1] - 2 = 0$, so that in particular the Cauchy distribution needs its own theoretical treatment or, at least, some limit considerations.

Remark 2.26. Definition 2.22 suggests the interpretation that two random quantities are called uncorrelated if they behave as if they were independent. This behaviour has been made precise in terms of the variation.

Remark 2.27. Linearity of the multivariate model is not sufficient to have $X + Y \sim F \in \mathcal{F}^d$ in Definition 2.22. As a well-known example, consider the set $\mathcal{F}$ of univariate Gaussian distributions with $H_\sigma(x) = \sigma x$, $\sigma \in \mathbb{R}$. Let $X \sim \mathcal{N}(0, 1)$ and $Y \sim \pi X$ where $\pi$ is a random sign, i.e., $\mathbb{P}(\pi = 1) = \mathbb{P}(\pi = -1) = 0.5$. Then, $Y \sim \mathcal{N}(0, 1)$, but the distribution of $X + Y$ does not belong to $\mathcal{F}$.

Remark 2.28. For two jointly $\alpha$-stable, scalar random variables $X$ and $Y$ with scale parameter $\sigma$ and $\tau$, respectively, the codifference is defined as (Samorodnitsky and Taqqu, 1994)

$$\tau_{X,Y} = [X] + [Y] - [X - Y]$$

and measures the difference between two variables. By way of contrast, $(\mathbb{[} + 1\mathbb{]} - 2)\langle X, Y \rangle = \mathbb{[} X + Y \mathbb{]} - (\mathbb{[} X \mathbb{]} + \mathbb{[} Y \mathbb{]})$ measures the difference in variation of a sum of two dependent variables and of two independent ones. Formally, $(\mathbb{[} + 1\mathbb{]} - 2)\langle X, Y \rangle = -\tau_{X, -Y}$.

Lemma 2.29. Let $(G, R, \mathcal{F}^d)$ be a multivariate model, $\mathbb{[} \mathbb{]}$ a variation and $\mathbb{[}1+1\mathbb{]} = 2$. Let $X$, $Y$ and $Z$ be random vectors such that their distributions and those of $X + Y$, $X + Z$ and $Z + Y$ are in $\mathcal{F}^d$. Let $\mu \in R$. Then, the following assertions hold:

$$\langle X, X \rangle = \mathbb{[} X \mathbb{]} \geq 0$$
$$\langle X, Y \rangle = \langle Y, X \rangle$$
$$\langle X, 0 \rangle = 0$$
$$\langle X + Z, Y \rangle = \langle X, Z + Y \rangle - \langle X, Z \rangle + \langle Z, Y \rangle$$
$$\langle X, X \rangle = 0 \Rightarrow X \equiv 0, \text{ if the variation is scale invariant}$$
$$\langle \mu X, \mu Y \rangle = \mathbb{[} \mu \mathbb{]} \langle X, Y \rangle, \text{ if the variation is scale invariant}.$$
2.6 Semi-metric between random vectors

The regression problem from classic PCA as given in (22) below is formulated using the squared $L^2$ distance, which is not a norm, but precisely fits the setting of a semi-metric $\rho$ measures the gap between two random variables $X, Y$.

A semi-metric is given by the following three conditions

\begin{align*}
\rho(X, Y) &\geq 0 \quad \text{(positivity),} \\
\rho(X, X) &= 0 \quad \text{(identity),} \\
\rho(X, Y) &= \rho(Y, X) \quad \text{(symmetry).} 
\end{align*}

With respect to the PCA we require further that $\rho$ is continuous and

\[ \rho\left(\sum_{i=1}^{2} \nu_i X_i, \sum_{i=1}^{2} \xi_i X_i\right) = \sum_{i=1}^{2} \rho(\nu_i X_i, \xi_i X_i), \quad \text{for } \nu_i, \xi_i \in \mathbb{R} \text{ and } X_1, X_2 \text{ indep.} \quad (15) \]

\[ \rho(X, Y) = \rho(U, V) \quad \text{for } X \equiv U \text{ and } Y \equiv V \quad \text{(a.s.)}. \quad (16) \]

Proposition 3.2 in Berg et al. [1984] deals with the generalization of a squared difference of real values towards complex values, in the framework of Hilbert spaces. The next definition carries over the implicit idea given there.

**Definition 2.30.** Let $(G, R, \mathcal{F}^d)$ be a multivariate model, $[\cdot]$ given by (11) and $[1 + 1] = 2$. For random vectors $X$ and $Y$ such that their distributions and that of $X + Y$ are in $\mathcal{F}^d$, let

\[ \rho(X, Y) := \|X\| + \|Y\| - 2\langle X, Y \rangle. \]

Then $\rho$ is called the associated semi-metric.

**Lemma 2.31.** Let $(G, R, \mathcal{F}^d)$ be a multivariate model, $[\cdot]$ a variation with $[1 + 1] = 2$, and $\rho$ be the associated semi-metric. Let $X$ and $Y$ be random vectors such that their distributions and that of $X + Y$ are in $\mathcal{F}^d$. Then, the following assertions hold:

\begin{align*}
\rho(X, X) &= 0 \quad \text{(identity),} \\
\rho(X, 0) &= \|X\| \quad \text{(17)} \\
\rho(X, Y) &= \|X + Y\| - [1 + 1] \langle X, Y \rangle = \frac{[1 + 1] ([\|X\| + \|Y\|] - 2 \|X + Y\|)}{[1 + 1] - 2} \quad (19) \\
\rho(X, Y) &= \|X\| + \|Y\| = \|X + Y\|, \quad \text{if } X \text{ and } Y \text{ are uncorrelated} \quad (20) \\
\rho(\mu X, \nu X) &> 0, \text{ if } \mu X + \nu X, (R, +) = (\mathbb{R}, +), [\mu] = |\mu|^\alpha, \text{ and } 0 < \alpha + 1. \quad (21) 
\end{align*}

Furthermore, Equation (15) holds. Now assume that the variation a vector is the sum of the variation of the components. Then, $\rho$ is well-defined on $\mathcal{F}^d_0$ if the representation of $X = \nu W \sim F_{\nu, \mu} \in \mathcal{F}^d_0$ is unique up to reordering of the summands. If $(R, +, \cdot) = (\mathbb{R}, +, \cdot)$ and $[\xi] = \xi^2$ then $\rho$ is well-defined if the representation is unique up to orthonormal transformations $U$ with $UW \sim W$ i.e., $X = (\nu U)(U^TW)$.
**Proof.** Equalities \((17)-(19)\) obviously hold. Inequality \((21)\) holds since \(\mu X \not\equiv \nu X\) implies \(X \not\equiv 0\) and then
\[
|\mu| \left| \nu \right| \alpha^2 \left| \alpha \right| \mu \left| \nu \right| \alpha^2 \left| \alpha \right| \mu = |\mu| \left( 1 + |\nu|^\alpha - 2(1 + |\nu|^\alpha) \right)
\]
with \(\xi = \nu/\mu\). The right-hand side takes its unique minimum at \(\xi = 1\), which is 0 due to \((17)\). Now, let \(R = \mathbb{R}\) and \(\|\xi\| = \xi^2\). For any orthonormal matrix \(U \in \mathbb{R}^{n \times n}\) we have \(X \equiv \nu U U^\top W\). Denote by \([\nu]\) the sum of the variation of all components of a matrix \(\nu\). Then,
\[
[\nu] = \text{tr}(\nu \nu^\top) = \text{tr}(\nu U U^\top \nu^\top) = \|\nu U\|.
\]
Note that, by Maxwell’s theorem ([Kallenberg, 2001], Proposition 12.2), \(UW \sim W\) holds for all orthonormal \(U\) if and only if the \(W_j\) are centered Gaussian.

### 3 Generalizing the classic PCA

In our model-based approach, the PCA is seen as an approximation of a random vector \(X\) with known distribution by some other random vector \(Y\) with a simpler structure. The function that maps a realization of \(X\) to a realization of \(Y\) is a projection in classic PCA. This function is called a reconstruction function here. We call a PCA inferable, if the existence and the knowledge of the reconstruction function is guaranteed. We start with reviewing the classic PCA.

#### 3.1 Classic PCA and Autoencoders

Classic PCA is usually understood as reducing the complexity of data in an optimal way with respect to the mean squared error. In general, the data is assumed to be an i.i.d. sample of \(X = (X_1, \ldots, X_m)\). Classic PCA is based on the solution of ([Pearson, 1901])

\[
\min_{H: \text{rank } H \leq p} \mathbb{E}\|X - HX\|_2^2.
\]

It can readily be seen, that \(H = V V^T\) is a solution to the minimization problem, where \(V\) is the matrix of the first \(p\) eigenvectors ([22]). In particular, \(H\) is a projection matrix, thus symmetric ([Baldi and Hornik, 1989]). In statistical literature, often \(H\) is replaced by \(VV^\top\) in ([22]), additionally assuming that \(V\) is orthonormal. To enforce uniqueness of the solution \(V\) in the general case, an ordering of the corresponding eigenvalues is further assumed.

This problem can be generalized as follows. Let \(L\) be a measurable loss function and \(\Theta\) an arbitrary parameter space with elements \((\theta_1, \theta_2) \in \Theta\) used to parametrize two measurable functions \(f_{\theta_1}\) and \(g_{\theta_2}\). Then, the autoencoder problem is given as

\[
\min_{(\theta_1, \theta_2) \in \Theta} \mathbb{E}[L(X, f_{\theta_1} \circ g_{\theta_2}(X))].
\]

Under mild assumptions, the existence of a solution is guaranteed.
Theorem 3.1. Let $X$ be a random variable and $\Theta$ a compact metric space for the parameter $\theta$ of the reconstruction functions $r_{\theta}: \Omega \rightarrow \Omega$. Let $L$ be a loss function that is bounded from below by $0$ and continuous for any function of one fixed argument. For all $x \in \Omega$, the map $r_{\theta}(x): \Theta \rightarrow \Omega$ be continuous. If for all $\theta \in \Theta$ it holds that
\[
\|L(X, r_{\theta}(X))\|_{L^\infty(\Omega, A, P)} := \text{ess sup} |L(X, r_{\theta}(X))| < \infty,
\]
then a solution to the autoencoder regression problem
\[
\min_{\theta \in \Theta} E[L(X, r_{\theta}(X))].
\]
exists.

Proof. The function $E[L(X, r_{\theta}(X))]: \Theta \rightarrow [0, \infty)$ has by assumption compact preimage, thus it suffices to show that it is continuous. For arbitrary $\theta \in \Theta$ and any sequence $(\theta_n)_{n \in \mathbb{N}}$ with limit $\theta$, we get by dominated convergence
\[
\lim_{n \to \infty} E[L(X, r_{\theta_n}(X))] = E[\lim_{n \to \infty} L(X, r_{\theta_n}(X))] = E[L(X, r_{\theta}(X))].
\]
This means that under reasonable choices of the statistical model and loss function we always have a solution to the autoencoder problem. We will go further in our approach and consider also
\[
\min_{\theta \in \Theta} E[L(X, Y_{\theta})]
\]
for certain classes of random variables $\{Y_{\theta}: \theta \in \Theta\}$.

3.2 Generalized PCA

Since the Hilbert space structure is given up here, various generalizations of the classic PCA are thinkable. We give four variants, which we consider particularly interesting. Two notions directly correspond to variable selection procedures in linear regression analysis. The following definition is based on a general semi-metric, although we have the associated semi-metric in mind, since there is no proved evidence that our suggested semi-metric should be preferred. The following definition allows that the PCA does not have a solution.

Definition 3.2. Let $(G, R, F^d)$ be a linear multivariate model and $\rho$ be a semi-metric such that \[\|\| \cdot \|\| \text{ hold. Let } F^d_0 \text{ be given as in Definition 2.14. Let } p \in \mathbb{N}, X = \nu W \sim F^d_{\nu, \mu} \in F^d_0 \text{ and } D((b_1, \ldots, b_p)) = \text{span } \{b_1, \ldots, b_p\} \text{ for } b_i \in R^d. \text{ For some closed } B \subset R^{d \times p} \text{ and some subset } I(X) = I(\nu_1, \ldots, \nu_n) \subset R^{d \times n}, \text{ the } p \text{-variate B-I PCA is defined as}
\]
\[
\text{PCA}_p(X) = \arg \min_{b \in B} \inf_{\xi \in D^n(b) \cap I(X)} \rho(X, \xi W).
\]
(25)

The PCA is called
1. exhaustive if \( B = R^{d \times p} \).

2. forward if

\[
B = \{ (b_1, \ldots, b_p) \in R^{d \times p} : (b_1, \ldots, b_{p-1}) \in \text{PCA}_{p-1}(X) \}. \tag{26}
\]

3. unrestricted if \( I = R^{d \times n} \).

4. (linearly) inferable if

\[
I(X) = I(\nu_1, \ldots, \nu_n) \subset \{ (H \nu_1, \ldots, H \nu_n) : H \text{ a (±-linear) map } R^d \to R^d \}. \tag{27}
\]

A set of vectors \( b_1, \ldots, b_p \) that is a solution to the \( p \)-variate PCA is called a set of first \( p \) principal vectors for \( F^d \nu, \mu \in F^d_0 \). Let \( F^d_n \in F^d_0 \) and \( b_{n,1}, \ldots, b_{n,p} \) be corresponding sets of principal vectors. If \( F^d_n \to_w F^d \in F^d \) and \( b_{n,i} \to b_i \in R^d \), then the set of vectors \( b_1, \ldots, b_p \) is called a set of first \( p \) principal vectors for \( F^d \in F^d \).

**Remark 3.3.** Condition (26) ensures that the principal vectors in forward PCA are in decreasing order of importance. If these principal vectors are orthogonal in a certain sense, they might be called eigenvectors. For instance, two vectors \( \mu, \nu \in R^d \) might be called orthogonal, if

\[
\langle \mu X, \nu X \rangle = 0 \quad \text{for all } F \in F \text{ and } X \sim F. \tag{28}
\]

Note that this is in general stronger than requiring \( \langle \mu, \nu \rangle = 0 \).

In the gaussian case, the vectors \( \mu \in R^d \) and \( \nu \in R^d \) are orthogonal in the sense of (28), if and only if they are orthogonal in the Euclidean sense. In the \( k \)-variate Gaussian case with \( d = 1 \), two matrices \( A, B \in R^{k \times k} \) are orthogonal if and only if \( AB^\top = 0 \), i.e., if the rows of \( A \) are all orthogonal to the rows of \( B \).

**Remark 3.4.** In some cases, it is sufficient to consider only \( n = 1 \) in the definition of a multivariate distribution, e.g., when adding independent variables is not reasonable. Then, Definition 3.2 still applies, if the operator \( \circ \) and all conditions built on it are ignored.

**Example 3.5.** (Continuation of the linear regression model, Example 2.12) Let \( P, S_\ell \) and \( L_\ell \) be defined as there, \( d \geq 1, 1 \leq m \leq \min\{k - 1, d\}, 1 \leq p \leq k - m \), and

\[
S_\ell^d = \{ (A, \ldots, A)^\top \in P^d : A \in S_\ell \}
\]

\[
S = \bigcup_{\ell = m+1}^{k} S_\ell^d,
\]

\[
B = S^p,
\]

Then the exhaustive PCA \( p \) searches the best subset selection with up to \( p \) predictor variables for a linear regression model with a \( d \)-variate dependent variable, \( k - m \) predictor variables, and \( m \) error variables. The forward PCA performs the forward selection.
Let us now consider some underlying structure of the variable selection. Let $k \geq 3$ and $C, D \in L_k$ with $C = C, D, 1 = D, 2 = D$ and $C, i = D, i = 0$, otherwise. Then, both equalities $C + AD = D$ and $D + AC = C$ are not solvable for $A \in L_k$. We say that $R = L_k$ is not strictly preordered. Since Theorem 3.7 of the Appendix is rather tight in its assumptions, which include strict preordering, we may expect that even the one-dimensional semimodule $L_1^k = L_k$ possesses subsemimodules with range larger than 1. This is indeed the case, as $CD \in S_\ell$ for $C \in L_k, D \in S_\ell$ and $\ell \leq k$. Then, span $\{S_{k-1}, S_k\}$ has rank 2, for instance. Assume, that two matrices $C, D \in L_k$ are orthogonal in the sense of (28). Then, it follows that either one of the corresponding linear regression models (i.e. the whole first line of the matrix) is identically zero, or both linear models are deterministic, i.e., $C, D = 0$, or both models are trivial, i.e., $C, D = D, D = 0$. Hence, we will not be able to orthogonalize the vectors that span the subspaces of the exhaustive PCA and the forward PCA. Therefore, we may not expect that forward PCA and exhaustive PCA will be the same, cf. Theorem 3.10 below.

Example 3.6. (Continuation of the linear regression model, Example 2.12) Other forms of variable selection are possible. For instance, let the subsemiring be given by the matrices

\[ A = \begin{pmatrix} A, A & A, D \\ 0_{(k-1)\times 1} & A, D \end{pmatrix}, \]

where $A, D$ is any matrix. For the PCA $p$ consider any matrix $A$ such that $A, 0 = 0$ and the last $k - 1 - p$ lines of $A, D$ are all zero. Further, the matrix $(A, D), (A, D)$ shall have the same rank as $A, D$. This approach balances out a good fit of the dependent variable with a good fit of the predictor variables. Therefore, we might consider it as a “PCA variable selection”. One extreme situation is that the variation puts nearly no weight on the dependent variable. Then, we end up primarily with a PCA for the predictor variables, in other words, with the PCA regression $\{\text{Jolliffe, 2002}\}$. On the other hand, if the variation puts no weight on the predictor variables (condoning that Condition (7) is violated), already PCA $1$ delivers exactly the standard regression.

Remark 3.7. For the linearly inferable PCA, matrices $H$ might be considered, whose so-called Barvinok rank is at most $p$, i.e., the set $I$ in Definition 3.2 is given by means of all matrices $H$ of the form $H, H, H, X \in R^{d \times p}$. Then, we may reformulate the exhaustive, linearly inferable PCA $p$ as

\[ \text{PCA}_p(X) = \arg\min_{H, H, X \in R^{d \times p}} \rho(X, H, H, X). \]

Hence, the optimization problem becomes a single $2pd$-dimensional problem. A further advantage is that this choice follows closely the autoencoder idea. A disadvantage is, that the Barvinok rank is rather restrictive, cf. Appendix A.2.

Remark 3.8. If the variation is scale invariant and $\rho$ is the associated semi-metric, then the exhaustive, unrestricted PCA reads

\[ \text{PCA}_p(X) = \arg\min_{b \in B} \sum_{j=1}^n \|\mu_j\| \]
with
\[ f_b(\nu_j), \quad f_b(u) = \min_{\xi \in D(b)} \left[ \frac{1}{1+1} \left( \|u\| + \|\xi\| \right) - 2 \frac{\|u + \xi\|}{1+1} \right], \quad u \in \mathbb{R}^d. \]

That is,
\[ \text{PCA}_p(X) = \arg \min_{\delta \in B} \int f_b(u) M(du), \quad M = \sum_{j=1}^n [\mu_j] \delta_{\nu_j}. \]

Remark 3.9. Except for the linearly inferable PCA, the requirement of the linearity of the multivariate model seems to be excessive, since only the univariate margins of \( X + \xi W \) enter in the associated semi-metric.

3.3 Coincidence of variants

Since the four variants of a generalized PCA coincide in the Gaussian case, we consider here general conditions for a coincidence in some exemplary cases.

Theorem 3.10. Let the conditions of Definition 3.3 hold with \( \rho \) the associated semi-metric and scale invariant variation. Assume that for any subsemimodules \( U \subset V \subset \mathbb{R}^d \) and \( m = \text{rank} V - \text{rank} U > 0 \), vectors \( b_1, \ldots, b_m \in \mathbb{R}^d \) exists such that \( V = \text{span} (U, b_1, \ldots, b_m) \). Assume that for any subsemimodule \( V \subset \mathbb{R}^d \) and \( \mu \in \mathbb{R}^d \) a vector \( \pi \in \mathbb{R}^d \) exists with the following two properties:

1. \( \text{span} (V, \pi) \supset \text{span} (V, \mu) \)

2. For all \( \nu \in \text{span} (V, \mu) \) and \( \xi \in \mathbb{R} \) a value \( \theta = \theta(\nu, \pi, \xi) \in \mathbb{R} \) and a \( \zeta \in V \) exists such that, for all \( \eta \in \mathbb{R}^d \) that are orthogonal to \( \pi \) in the sense of (28), we have

\[ \nu + \eta + \xi \pi = \zeta + \eta + \theta \pi \]

(29)

\[ \nu + \eta \text{ and } \theta \pi \text{ are orthogonal.} \]

(30)

Then the unrestricted, forward PCA coincides with the unrestricted, exhaustive PCA. If equality holds in (27) and \( \pi \) has always a representation of the form \( \pi = \nu^* + \xi^* \mu \) with \( \nu^* \in V \) and \( \xi^* \in \mathbb{R} \), then the linearly inferable, forward PCA coincides with the linearly inferable, unrestricted PCA.

Proof. Condition (29) ensures that a sequence of principal vectors \( b_1, \ldots, b_p \) can be replaced by a sequence of pairwise orthogonal vectors \( b_1^0, b_2^0, \ldots, b_p^0 \), so that \( \text{span} (b_1, \ldots, b_k) \subset \text{span} (b_1^0, b_2^0, \ldots, b_k^0) \) for all \( k = 2, \ldots, p \). Let \( M_k^* \) be the minimum in (25) for \( D^n := U_k := \text{span} (b_1^0, \ldots, b_k^0) \). Then \( M_k^* \) is decreasing and \( M_k^* - M_{k-1}^* \) only depends on \( b_k^0 \). Now, consider the unrestricted exhaustive PCA. Let \( V_k \) be the space spanned by the principal vectors \( c_1, \ldots, c_k \). Condition (29) ensures that pairwise orthogonal \( c_1^0, \ldots, c_p^0 \) of \( V_p \) exists such that either \( c_1^0 = b_1^0 \) or \( c_1^0 \) is orthogonal to \( U_p \) in the sense of (28). We may assume further, that those vectors that are orthogonal to \( U \) are ordered according to the rules of a forward PCA. Let \( M_k^* \) be the minimum in (25) for \( D^n := \text{span} (c_1^0, \ldots, c_k^0) \). Again, \( M_k^* \) is decreasing and \( M_k^* - M_{k-1}^* \) only depends on \( c_k^0 \). Let \( M_0^* := M_0^* := 0 \). Assume the two
sequences \((M_k^r - M_{k-1}^r)_{k=1}^p\) and \((M_k^s - M_{k-1}^s)_{k=1}^p\) are identical. Let the spaces \(V_i\) and \(U_i\) be identical up to \(k-1\), but \(V_k \neq U_k\). Then \(M_k^r - M_{k-1}^r = M_i^r - M_{i-1}^r\) for \(i = k+1, \ldots, p\). This can be seen as follows. Let \(i\) smallest such that \(M_k^r - M_{k-1}^r > M_i^s - M_{i-1}^s\). As \(V_k \neq U_k\) a vector \(v \in V_i\) exists that is orthogonal to \(U_p\). Replacing \(b_i^0\) by \(c_k^0\) gives a contradiction to \(b_k\) being an optimal choice. Now assume that the sequences are different. Then \(k \in \{1, \ldots, p\}\) exists such that \(M_k^r - M_{k-1}^r < M_k^s - M_{k-1}^s\). Replacing \(b_k\) by \(c_k\) leads to a contradiction as before. In case of linearly inferable PCA, the additional condition ensures that \(\pi\) can be represented by means if a \(d\)-linear map if \(\nu\) and \(\mu\) do so. Except that the proof is the same as in the exhaustive case.

Consider the following counterexample for \((G, \vee, \cdot)\). Let \(X = (2, 1)\)\(^T\) \(W_1 \vee (1, 2)\)\(^T\) \(W_2\) with \(W_1 \sim F_1\). A principal vector for the unrestricted PCA with \(k = 1\) cannot be a multiple of any of the two unit vectors. Hence, the forward, unrestricted PCA for \(k = 2\) is different from the exhaustive one.

The coincidence of forward PCA with exhaustive PCA in the above theorem needs structural assumptions on the space \(\mathbb{R}^d\), essentially the existence of a genuine scalar product. The coincidence of the unrestricted PCA with the linearly inferable PCA needs assumptions on the distribution. A trivial sufficient condition is that a \(d\)-linear map \(A\) (depending on \(X\) itself) exist such that \((W_1, \ldots, W_n)^T = AX\).

### 4 Example: max-stable distributions

For \(\alpha > 0\), the univariate \(\alpha\)-Fréchet margins \(F_\lambda^{(\alpha)}\), \(\lambda > 0\), is given by

\[
F_\lambda^{(\alpha)} = 1_{(0, \infty)}(x)e^{-(\lambda/x)^\alpha}, \quad x \in \mathbb{R}.
\]

Stoev and Taqqu (2003) call \(\lambda\) the scale coefficient and define \(\|X\|_\alpha := \lambda\) for \(X \sim F_\lambda^{(\alpha)}\).

For two independent random variables \(X_\lambda \sim F_\lambda^{(\alpha)}\) and \(X_\mu \sim F_\mu^{(\alpha)}\), we have \(X_\lambda \vee X_\mu \sim F_{\lambda \vee \mu}^{(\alpha)}\) with \(\lambda \circ \mu = (\lambda^\alpha + \mu^\alpha)^{1/\alpha}\). Hence, \(\|X\|_\alpha\) is indeed a metric. Proposition 2.6 in Stoev and Taqqu (2003) shows that the associated semi-metric \(\rho\) is indeed a metric.

Let \(F_0^{(\alpha)}(x) = 1_{[0, \infty)}(x)\). Then \(\nu X_\lambda \vee \mu X_\lambda = (\nu \vee \mu)X_\lambda\) and \(\nu(\lambda \circ \mu) = \nu \lambda \circ \nu \mu\) for \(\lambda, \mu, \nu > 0\). Hence, \((G, R, \mathcal{F}_d)\) is a linear multivariate model for \((G, \vee)\) and \((R, \vee, \cdot)\) with \(G = R = [0, \infty)\). In the light of Stoev and Taqqu (2005), Definition 2.14 deals with an extremal integral over a discrete measure with finite support, where the typically infinite index set \(T\) of a stochastic process is replaced by a finite one, \(T = \{1, \ldots, d\}\).

For ease, consider henceforth the case \(\alpha = 1\) only. Then, the set of all \(d\)-variate max-stable distributions \(F\) with Fréchet margins are given by Stoev and Taqqu (2003; Beirlant et al., 2004)

\[
- \log F(x) = \int_\Xi \sum_{i=1}^d \frac{u_i}{x_i} S(du), \quad x = (x_1, \ldots, x_d) \in (0, \infty)^d,
\]

where \(\Xi := \{u \in [0, \infty)^d : \|u\|_q = 1\}\) for some \(q \geq 1\) and the so-called spectral measure \(S\).
satisfies
\[ \int_{\Xi} u_i S(du) = \lambda_i, \quad i = 1, \ldots, d. \]
Here, \( \lambda_i > 0 \) is the scale coefficient of the \( i \)-th component. Let \( X = \nu W \sim F_{\nu, \mu}^{(\alpha)} \in \mathcal{F}_0^d \). Without loss of generality let \( \sum_{i=1}^d \nu_{ij} = 1 \) for all \( j \in \{1, \ldots, n\} \), i.e., \( \|\nu_j\|_\infty = 1 \) for \( \nu_j = (\nu_{ij}, \ldots, \nu_{ij}) \). Then, for \( x \in (0, \infty)^d \), we have
\[
\mathbb{P}(X \leq x) = \mathbb{P}(\nu_j W_j \leq x_j, i = 1, \ldots, d; j = 1, \ldots, n) = \exp \left( - \sum_{j=1}^n \sum_{i=1}^d \frac{\nu_{ij} \mu_j}{x_i} \right) = \exp \left( - \sum_{i=1}^d \sum_{j=1}^n \frac{u_i}{x_i} S_{ij}(du) \right)
\]
with
\[ S_{ij} = \sum_{j=1}^n \|\nu_j\|_q \mu_j d_j / |\nu_j|_q, \]
such that
\[ \lambda_i = \int_{\Xi} u_i S_{ij}(du) = \sum_{j=1}^n \nu_{ij} \mu_j, \quad i = 1, \ldots, d. \]
We get for \( f_b \) in Remark 3.8
\[ f_b(u) = \min_{\xi \in D(b)} (2 \|u + \xi\| - \|u\| - \|\xi\|). \]
Let \( \nu W \sim F_{\nu, \mu}^{(\alpha)} \). If the variation of vector is defined as the sum of the variation of the components, then we have \( \int \nu W = \sum_{i=1}^d \sum_{j=1}^n \nu_{ij} \mu_j = \sum_{i=1}^d \lambda_i < \infty \) and
\[ f_b(u) = \min_{\xi \in D(b)} \|u - \xi\|_1. \]
As \( f_{cb} = f_b \) for \( c > 0 \) and \(((0, \infty), \cdot, \cdot)\) is a group, the exhaustive, unrestricted PCA reads
\[ \text{PCA}_p(X) = \arg \min_{b \in B, \|b\|_q \leq 1} \int_{\Xi} f_b(u) S_{ij}(du). \]
Since \( f_b(u) \leq \|u\|_1 \) and hence \( 0 \leq \int_{\Xi} f_b(u) S_{ij}(du) \leq \sum_{i=1}^d \lambda_i \), the solution to the PCA problem is not empty, cf. Theorem 3.1. Assume \( S_{\nu_n} \to S_\infty \) in the weak topology. Let \( b_n \in B \) with \( \|b_n\|_q \leq 1 \) be respective solutions. Since \( \{b \in B : \|b\|_q \leq 1\} \) is a compact set, we have \( b_{n_i} \to b_\infty \in B \) with \( \|b_\infty\|_q \leq 1 \) for a subsequence \( (n_i) \). Now, \( \Xi \) is also a compact set and \( f_b(u) \) is continuous in \( u \) and \( b \). Then, the function \( (b, u) \mapsto f_b(u) \) is uniformly continuous and a constant \( C \geq 0 \) exists such that
\[ \int_{\Xi} f_{b_{n_i}}(u) S_{\nu_i}(du) \to C \quad (i \to \infty). \]
We get \( \int_{\Xi} f_{b_\infty}(u) S_{\infty}(du) = C \) by standard arguments. Similarly,
\[ \arg \min_{b \in B, \|b\|_q \leq 1} \int_{\Xi} f_b(u) S_{\infty}(du) \geq C. \]
Hence, for any spectral measure $S$, the exhaustive, unrestricted PCA problem equals

$$\text{PCA}_p(X) = \arg \min_{b \in B, |b| \leq 1} \int_\Xi f_b(u)S(du).$$

The alternative choice $[uW_\xi] := \|u\|_\infty \xi$ for $u \in R^d$ and $W_\xi \sim F_\xi$, looks appealing, since then the variation yields the extremal coefficient,

$$[\nu W] = \sum_{j=1}^n \mu_j \bigg[ \sum_{i=1}^d \nu_{ij} \bigg] = \int_\Xi \bigg[ \sum_{i=1}^d u_i S_\nu(du) \bigg],$$

but then

$$f_b(u) = \min_{\xi \in D(b)} \|u\|_\infty - \|\xi\|_\infty$$

becomes pathological.

### 5 Discussion

120 years ago, (Pearson, 1901) introduced the PCA to simplify the structure of data. At that time, statistical models were unknown. Surprisingly, up to date, not much attempt has been made to substantiate the PCA by some theoretical framework. With our original aim to define a PCA rigorously for extreme values we suggest here a general model, where the classic PCA reappears as the Gaussian case. Knowing from this paper, that only a narrow family of distributions suits for construction, it is even more challenging to understand theoretically, why PCA is that successful, in particular, when the assumptions are not satisfied.

Linear regression models fit our framework and the PCA delivers the theoretical basis for variable selection. Three points are remarkable. First, variable selection splits up into two parts (as our PCA does in general): (i) estimation of the underlying model; (ii) approximation of the estimated model by a simpler model. Second, the predictor variables together with a scalar dependent variable build a single vector-valued quantity. Hence, the PCA acts on a formally univariate quantity, and the approximation takes place on a complex subspace structure of a one-dimensional space. From this point of view, it is not surprising, when the results of the various variable selection procedures are difficult to compare. Third, the difference between the error term and a scalar dependent variable vanishes formally, as the latter takes the place of the first, see Equality (3).

The set $B$ in the Definition 3.2 of the generalized PCA corresponds to the hidden layer of a standard autoencoder. Two generalizations are introduced in Definition 3.2. The set $I$ refers to modifications of a standard autoencoder that are common to neural networks. The genuinely novel idea that is introduced into neural network modeling is the following, though. The sum that enters the (sigmoid) activation function is replaced by some other semigroup operation. From a modeling point of view for neural networks, this paper can be seen as a guideline for choosing such semigroup operations, in particular in heterogeneous networks (Piras et al., 1996). Indeed, recent papers show that the
latter can be much more efficient than homogeneous networks (She et al., 2021), in particular in a complex, space-time context (Christou et al., 2019). For instance, the brain seems to consist of various classes of neurons, which process data markedly differently (Stefanescu and Jirsa, 2008; Schliebs et al., 2009).

Classic PCA and many extensions thereof approximate data by a lower dimensional hyperplane in the real space. In our approach, we define a multivariate distribution by means of a spectral representation. Hence, our generalized PCA can be interpreted as searching a best “hyperplane” approximation in a kind of Fourier space. This contrasts in particular the approaches so far for extreme values (Jiang et al., 2020; Drees and Sabourin, 2021). The so-called spectral PCA (Thornthill et al., 2002) is somehow close to our approach, but sticks to the idea of classic PCA: data of stationary processes are first Fourier transformed, before they enter the classic PCA.

The foundation of our generalized PCA on semi-groups made a workaround for the mean squares of the residuals in classic PCA necessary. As a side effect, hitherto existing approaches can be seen in a different light. For instance, the scalar product for random variables includes operations from three different semi-groups, which coincide in the standard (i.e. Gaussian) case. Further, scaling parameters carry the structural information, not the random variables. Finally, the variance is a theoretically convenient quantity, but lacks an intuitive statistical interpretation — being the square of a nicely interpretable quantity is not satisfying. The variation of Definition 2.17, however, has a nice practical interpretation, as it measures the amount of randomness. The variance is now the (unique) specification of the variation in case of Gaussian random variables.

Our approach includes various open questions. Obvious ones are the uniqueness of the PCA outside trivially equivalent representations, the specification of the inferable PCA, and the computation in reasonable time. Finally, a slight extension of the current approach will be needed to perform a PCA that is adapted to discrete distributions.

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A An algebraic excursion: ranks

The change from spaces based on a field to spaces based on a semiring is drastic. For instance, the dimension of a semimodule is generally not well defined, i.e., bases with different cardinalities might span the same space (Golan, 1999). Therefore, the rank, i.e. the minimal cardinality of all sets of vectors that span the space, is considered, see Definition 2.5. Furthermore, the rank of a subsemimodule might be greater than the rank of the semimodule itself. This may happen even if the rank of the semimodule equals one. A simple example is given by the semiring \((\mathbb{N}_0, +, \cdot)\) and the subsemimodule
\( \mathbb{N}_0 \setminus \{1, 2, 4, 7\} \) over \( \mathbb{N}_0 \), spanned by the one-dimensional vectors 3 and 5. The unique rank of a matrix in a Hilbert space context splits up into various definitions in a semiring context (Appendix A.2).

**Definition A.1.** A semiring \((R, +, \cdot)\) is called a semifield if \( R \) is division free and \((R, \cdot)\) is commutative. A semifield \((R, +, \cdot)\) is called **proper**, if \((R, +)\) is a group.

Various definitions of the notion “independence”, hence of a basis of a semimodule, are given in literature (Gondran and Minoux, 1984, Def 2.2.5). We follow here Definition 2.2.2 in Wagneur (1991).

**Definition A.2.** Let \( S \) be a semimodule over a semiring \((R, +, \cdot)\). A set of vectors \( \{x_i \in S : i \in I\} \) indexed by the set \( I \), is called independent (or non-quasi-redundant), if for all finite subsets \( I_0 \subset I \), all \( k \in I_0 \) and all \( \alpha_i \in R \) and \( \gamma \in R \setminus \{0\} \) we have

\[
\sum_{i \in I_0 \setminus \{k\}} \alpha_i x_i \neq \gamma x_k.
\]

(31)

In case \((R, \cdot)\) is an abelian group, \( \gamma \) in condition (31) can be chosen to be 1, i.e., condition (31) is equivalent to

\[
\sum_{i \in I_0 \setminus \{k\}} \alpha_i x_i \neq x_k,
\]

(32)

cf. Gondran and Minoux (1984).

**Definition A.3.** Let \( S \) be a semimodule over a semiring \( R \). If \( B \subset S \) is a set of independent vectors and if all \( x \in S \) have a representation

\[
x = \sum_{b \in B} \alpha_b b, \quad \alpha_b \in R,
\]

then \( B \) is called a (semi-)basis of \( S \). If, for all bases \( B \) of \( S \), we have \( \#B = \text{rank} S \), then \( \text{rank} S \) is called the **dimension** of \( S \).

### A.1 Rank of a subsemimodule

Exemplarily and in particular with respect to the PCA for extreme values, we show here that we have a radical change of the behaviour of random vectors from dimension \( d = 2 \) to dimension \( d = 3 \) if we consider a genuine semiring instead of a field.

**Definition A.4.** Let \( G \) be a semigroup and \( \alpha, \beta \in R \). We write \( \alpha \preceq \beta \), if \( \gamma \in G \) exists, such that \( \alpha + \gamma = \beta \). We call \( G \) (canonically) preordered if for all \( \alpha, \beta \in G \) we have \( \alpha \preceq \beta \) or \( \beta \preceq \alpha \).

**Definition A.5.** Let \( R \) be a semiring and \( \alpha, \beta \in R \). We write \( \alpha \preceq \beta \), if \( \gamma \in R \) exists, such that \( \alpha + \gamma \beta = \beta \). We call \( R \) strictly preordered if for all \( \alpha, \beta \in R \) we have \( \alpha \preceq \beta \) or \( \beta \preceq \alpha \).
Lemma A.6. Let \( R \) be a strictly preordered semiring, \( S = R^2 \) and \( x_i = (x_{i1}, x_{i2}) \in S \) for \( i \in I := \{1, 2, 3\} \). Then a permutation \( \pi \) on \( I \) and \( k \in \{0, 1\} \) exists, such that

\[
\begin{align*}
  x_{\pi(1),2-k} \cdot x_{\pi(3),1+k} & \leq x_{\pi(1),1+k} \cdot x_{\pi(3),2-k} \\
  x_{\pi(2),1+k} \cdot x_{\pi(3),2-k} & \leq x_{\pi(2),2-k} \cdot x_{\pi(3),1+k}.
\end{align*}
\]  

(33)

Proof. Without loss of generality we may assume that

\[ x_{12} x_{31} \leq x_{11} x_{32}. \]

If \( x_{21} x_{32} \leq x_{22} x_{31} \) choose \( \pi = c(1,2,3) \) and \( k = 0 \). Otherwise we distinguish two cases:

(i) if \( x_{11} y_{22} \leq x_{12} x_{21} \) then choose \( \pi = c(2,3,1) \) and \( k = 0 \) as \( x_{12} x_{31} \leq x_{11} x_{32} \) holds true;
(ii) \( x_{22} x_{31} \leq x_{21} x_{32} \) and \( x_{12} x_{21} \leq x_{11} y_{22} \) hold; choose \( \pi = (3,1,2) \) and \( k = 1 \) here.

Theorem A.7. Let \( S \) be a semimodule over a semifield \( R \). If \( V \subset S \) is a subsemimodule with rank equal to \( 0 \) or \( 1 \), then the dimension of \( V \) exists. If \( R \) is additionally strictly preordered and \( d \leq 2 \), then any subsemimodule of \( R^d \) has rank at most \( d \).

Proof. For \( V = \{0\} \) the assertions are obvious. Let \( \text{rank}(V) = 1 \) and let \( x \in V \) be a basis vector. Assume \( v, w \in S \) are two distinct elements of another basis of \( V \). Then \( \alpha, \beta \in R \setminus \{0\} \) exist such that \( v = \alpha x \) and \( w = \beta x \). Hence, \( \beta v = \alpha w \), a contraction to the independence assumption.

Let \( \text{rank}(V) = 2 \) and assume \( x = (x_1, x_2), y = (y_1, y_2), z = (z_1, z_2) \) are elements of a basis of \( V \). Lemma A.6 yields that, without loss of generality,

\[
\begin{align*}
  x_1 z_2 & = x_2 z_1 + \alpha_{xz} x_1 z_2 \\
  y_2 z_1 & = y_1 z_2 + \alpha_{zy} y_2 z_1
\end{align*}
\]

(34) (35)

for some \( \alpha_{xz}, \alpha_{zy} \in R \setminus \{0\} \). Indeed, the value 0 is excluded due to the independence assumption. We distinguish three cases: (i) one of the components of \( x, y, \) or \( z \) equals 0;
(ii) none of the components equals 0 and a permutation of \( x, y \) and \( z \) and the indices of the component exist such that the conditions (34) and (35) hold, but not

\[
a_{zy} x_2 z_1 + \alpha_{xz} x_1 z_2 = 0;
\]

(36)

(iii) none of the components equals 0 and conditions (34)–(36) holds for some permutation.

• Without loss of generality let us assume that \( x_1 = 0 \). The assumption that \( x_2 y_1 z_1 = 0 \) directly contradicts the assumption of semi-linear independence. So we may assume \( x_2 y_1 z_1 \neq 0 \). Furthermore we may assume that \( z_1 y_2 \leq y_1 z_2 \). Then \( \alpha \in R \) exists such that \( z_1 y_2 + \alpha y_1 z_2 = y_1 z_2 \). Then we have

\[
\alpha y_1 z_2 \begin{pmatrix} 0 \\ x_2 \end{pmatrix} + x_2 z_1 \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = x_2 y_1 \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}.
\]

This is a contradiction to the assumed independence.
Let $\alpha = \alpha_{xy}z_1$ and $\beta = \alpha_{xz}x_1z_2$. If (36) does not hold then $\alpha x_1 x_2 + \beta x_1 y_2 \neq 0$ and we get a contradiction to the independence of $x, y, z$ by

$$(\alpha x_2 z_1 + \alpha \beta) \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} + \beta x_1 z_2 \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = (\alpha x_1 x_2 + \beta x_1 y_2) \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}.$$ 

Equality (36) implies

\[
\begin{align*}
\alpha_{xy} z_1 \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} + \alpha_{xz} x_1 \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} &= x_1 z_1 \begin{pmatrix} \alpha_{xy} + \alpha_{xz} \\ 0 \end{pmatrix} \\
\alpha_{xz} z_2 \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} + \alpha_{zy} x_2 \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} &= x_2 z_2 \begin{pmatrix} 0 \\ \alpha_{zy} + \alpha_{xz} \end{pmatrix}.
\end{align*}
\]

The assumption $\alpha_{xy} + \alpha_{xz} = 0$ contradicts the assumption that $x$ and $z$ are independent. Hence, $x_1 x_2 z_1 z_2 (\alpha_{xy} + \alpha_{xz}) y \neq 0$ and can be represented by a $+$-linear combination of $x$ and $z$.

Even if $R$ is strictly preordered, a $d$-dimensional subsemimodule $V \subset R^d$ can be a genuine subset.

As usual, $\delta^i$ denotes the $i$-fold product of $\delta \in R$.

**Theorem A.8.** Let $S = R^3$ be a semimodule over a semifield $R$ and $n \in \mathbb{N} \cup \{\infty\}$. Assume that $\delta \in R$ exists such that the following condition holds true:

$$\gamma \delta^i > \gamma \beta \quad \text{for all } 1 \leq i < n + 1, \gamma, \beta \in R, \gamma \neq 0, \beta \neq 0$$

Then a subsemimodule $V \subset S$ exists with $\operatorname{rank} V \geq n$.

Roughly speaking, condition (37) requires the existence of a number $\delta > 1 + 1$. This is true for the maximum semifield $([0, \infty), \lor, \cdot)$, where (37) holds for all $n \in \mathbb{N}$. If $R$ is a proper semifield, then condition (37) is void.

**Proof.** We may assume that $n$ is finite and define $x_i = (1, \delta^i, \delta^{2i})$ for $1 \leq i \leq n$. In order to show that

$$\sum_{i \neq j} \alpha_i x_i \neq \gamma x_j$$

for all $1 \leq j \leq n$, $\alpha_i \in R$ and $\gamma \in R \setminus \{0\}$, it suffices to show that for all $1 \leq j \leq n$ and $\gamma \in R \setminus \{0\}$ the two equalities

$$\sum_{i \neq j} \alpha_i = \gamma$$

and

$$\sum_{i \neq j} \alpha_i \delta^i = \gamma \delta^j$$

(38) and (39)
imply
\[ \sum_{i>j} \alpha_i\delta^{2i} \leq \gamma\delta^{2j}. \quad (40) \]

Note that (37) implies
\[ \delta^j > \delta^i \text{ for } 0 \leq i \leq j < n + 1. \quad (41) \]

Definition A.4 immediately yields
\[ \alpha \leq \beta \implies a\gamma \leq \beta\gamma \text{ for all } \gamma \in R \quad (42) \]
\[ \alpha \leq \beta, \gamma \leq d \implies a\gamma \leq \beta\gamma \text{ for all } \gamma \in R \quad (43) \]

Now assume that \( \sum_{i>j} \alpha_i\delta^{2i} \leq \gamma\delta^{2j} \). Then equality (39) and calculation rules (41)–(43) yield
\[ \gamma\delta^{2j+1} = \delta^{j+1} \left( \sum_{i>j} \alpha_i\delta^i + \sum_{i<j} \alpha_i\delta^i \right) \leq \sum_{i>j} \alpha_i\delta^{2i} + \sum_{i<j} \alpha_i\delta^{i+j+1} \leq \gamma\delta^{2j} + \delta^{2j} \sum_{i<j} \alpha_i \leq (\gamma + \gamma)\delta^{2j} \]

In total, this chain of inequalities contradicts condition (37), so that \( \sum_{i>j} \alpha_i\delta^{2i} \leq \gamma\delta^{2j} \) holds true.

A.2 Rank of a matrix

Let \( H : R^d \to R^d \) be a \( \dagger \)-linear map. From the point of view of a PCA, we expect that \( H \) does not enter into a linearly inferable “p-dimensional” PCA_p, if \( \text{im } H \subset \text{span} \{b_1, \ldots, b_p\} \) for all vectors \( b_1, \ldots, b_p \in R^d \). This basic requirement is ensured by the definition of the set \( B \) in Definition 3.2 of a PCA.

The unique rank of a matrix in standard linear algebra splits into different notions already in the tropical algebra (Akian et al., 2006; Maclagan and Sturmfels, 2013). We call a matrix \( M \in R^{k \times d} \) tropical, if \( R = ((0, \infty), \cdot, \cdot) \). Akian et al. (2006) and Guterman and Shitov (2016) give overviews over various rank definition for a tropical matrix, most of them can be immediately generalized to arbitrary semirings \( R \). For instance, the row rank and the column rank can be defined using any of the definitions of independence. A stronger form of Definition A.2 leads to ranks in the so-called Gondran–Minoux sense. The so-called tropical rank is frequently used. Its definition is more complex, but the tropical rank can be interpreted as the dimension of the tropical linear span (Guterman and Shitov, 2016). The Kapranov rank has a convenient interpretation of the least dimension of a tropical linear space that includes the rows (columns) of \( M \). The Barvinok rank, or factor rank, is the smallest \( r \), such that
\[ M = H_1H_2^\top, \quad H_1 \in R^{k \times r}, H_2 \in R^{r \times d}. \]
Various relations between the different notions of a rank exist. For example, the tropical rank is less than or equal to the Kapranov rank, which is itself less than or equal to the Barvinok rank. However, they do not bound each other, in general (Kim and Roush, 2006).

The determination of the rank of a matrix is typically an NP hard problem, see Guterman and Shitov (2016). In some cases, it is even undecidable (Kim and Roush, 2006). The problem to determine whether the rank is less than or equal to a given number, is, in general, polynomial, i.e., much simpler. The construction in Remark 5.3 even guarantees immediately that the Barvinok rank is at most $p$.

Note that our approach of a PCA is different from the so-called tropical PCA, which is a purely geometrical approach leading to a different optimization problem (Page et al., 2020).

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