CONVEX COMBINATION OF DATA MATRICES: PCA PERTURBATION BOUNDS FOR MULTI-OBJECTIVE OPTIMAL DESIGN OF MECHANICAL METAFILTERS

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Abstract. In the present study, matrix perturbation bounds on the eigenvalues and on the invariant subspaces found by principal component analysis is investigated, for the case in which the data matrix on which principal component analysis is performed is a convex combination of two data matrices. The application of the theoretical analysis to multi-objective optimization problems – e.g., those arising in the design of mechanical metamaterial filters – is also discussed, together with possible extensions.

1. Introduction. Principal Component Analysis (PCA) is a well-known data dimensionality reduction technique. It works by projecting a dataset of $m$ column vectors $\mathbf{x}_j \in \mathbb{R}^n$, $j = 1, \ldots, m$ (represented by a data matrix $\mathbf{X} \in \mathbb{R}^{m \times n}$, whose rows are the transposes of such column vectors) onto a reduced $d$-dimensional subspace of $\mathbb{R}^n$, which is generated by the first $d < n$ so-called principal directions. These are orthonormal eigenvectors of the symmetric and positive semi-definite PCA matrix.

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The reader is referred to [11, Chapters 1-3 and 6] for a presentation of the main properties of PCA, and to [13, Chapter 4] for a shorter introduction to the topic, in which all the main algebraic and geometric properties of PCA are proved mainly for the case of centered datasets. Nevertheless, most of their proofs can be easily extended to the case of uncentered datasets, which are mainly considered in the present article.
\( C = \frac{1}{n} X^T X \in \mathbb{R}^{n \times n} \) (where the symbol \( ^\top \) denotes transposition), which are associated with its \( d \) largest positive eigenvalues. The latter are proportional (via the multiplicative factor \( \frac{1}{n} \)) to the \( d \) largest positive eigenvalues of the related symmetric and positive semi-definite Gram matrix \( G = XX^\top \in \mathbb{R}^{m \times m} \), whose element in position \((i,j)\) is the inner product between the vectors \( x_i \) and \( x_j \). Focusing on such eigenvalues is important because the eigenvalues corresponding to discarded principal directions (the ones associated with the successive eigenvalues, not selected by PCA) provide information about the mean squared error of approximation of the dataset when only the first \( d \) principal directions and corresponding principal components (i.e., the projections of the data vectors \( x_j \) onto each such principal direction) are kept to construct that approximation. As a consequence, knowing these eigenvalues is useful also to select a suitable value for \( d \). Another important property of PCA is that, among all subspaces of \( \mathbb{R}^n \) having dimension \( d \), the one generated by the first \( d \) principal directions found by PCA minimizes the mean squared error of approximation of the dataset. Moreover, when the dataset has zero mean, each eigenvalue of the PCA matrix represents the empirical variance of the projection of the dataset onto the corresponding principal direction.

Given this framework, the goal of this article is first to get a matrix perturbation bound on the eigenvalues of the Gram matrix \( G \), then a matrix perturbation bound on the corresponding principal directions (and more generally, on the set of invariant subspaces) of the related PCA matrix \( C \), for the case in which the data matrix \( X \) is a convex combination of other two data matrices. According to the authors’ experience, this is a non-standard, unexplored, but potentially quite interesting way of using PCA in connection with multi-objective optimization (a framework in which a convex combination of two data matrices can arise quite naturally). The application of the theoretical analysis to multi-objective optimization is discussed extensively in the article, together with possible extensions of such theoretical analysis. In more details, the cases of unconstrained multi-objective maximization with quadratic and concave objective functions [1] and of the multi-objective optimal design of metamaterial filters [19, 2] are investigated.

The article is organized as follows. Section 2 provides a matrix perturbation bound on the eigenvalues found by PCA when the latter is applied to the convex combination of two data matrices. This section reports an extension of the analysis made by the authors in [7]. Section 3 provides a similar matrix perturbation bound related to the angles between corresponding principal directions (but also to suitably-defined angles between invariant subspaces associated to subsets of these principal directions). Section 4 presents a simple numerical example of application of the bounds obtained in the two sections above. Section 5 investigates theoretically one situation for which it makes sense to apply PCA to the convex combination of the two datasets, i.e., the case of multi-objective optimization solved by the weighted sum method, for which the dataset is the convex combination of two sampled gradient fields. First, the simple case of unconstrained multi-objective maximization with quadratic and concave objective functions is theoretically investigated, then the application to the multi-objective optimal design of mechanical metamaterials is discussed, in connection with other recent works written by the authors. Finally, Section 6 discusses possible developments, together with other applications.
2. Matrix perturbation bound on the eigenvalues of the Gram matrix associated with a convex combination of two data matrices. In this section, a perturbation bound on the eigenvalues of the Gram matrix of a dataset is provided, for the case in which its data matrix \( X(\alpha) \) is a convex combination of two data matrices \( X_1 \) and \( X_2 \), with varying weights \( \alpha \in [0, 1] \) and \( 1 - \alpha \), respectively.

In order to state the next proposition, the following notation is introduced. Let \( X_1, X_2 \in \mathbb{R}^{m \times n} \) be two data matrices, \( \alpha \in [0, 1] \), \( G(\alpha) = X(\alpha)X^\top(\alpha) \in \mathbb{R}^{m \times m} \) be the Gram matrix of their convex combination \( X(\alpha) \triangleq \alpha X_1 + (1 - \alpha) X_2 \) with weights \( \alpha \) and \( 1 - \alpha \), \( K \in \mathbb{N} \) and, for \( k = 0, 1, \ldots, K \), \( \alpha_k \triangleq \frac{k}{K} \). Let the non-negative eigenvalues of \( G(\alpha) \) and \( G(\alpha_k) \) be ordered non-increasingly, respectively, as \( \lambda_1(G(\alpha)) \geq \lambda_2(G(\alpha)) \geq \ldots \geq \lambda_m(G(\alpha)) \) and \( \lambda_1(G(\alpha_k)) \geq \lambda_2(G(\alpha_k)) \geq \ldots \geq \lambda_m(G(\alpha_k)) \). Finally, let \( \sigma_1(X(\alpha)) \) and \( \sigma_1(X(\alpha_k)) \) be the largest singular values of \( X(\alpha) \) and \( X(\alpha_k) \), respectively.

**Proposition 1.** For any \( k = 0, 1, \ldots, K - 1 \) and \( \alpha \in [\alpha_k, \alpha_{k+1}] \), the following holds, for all \( i = 1, \ldots, m \):

\[
|\lambda_i(G(\alpha)) - \lambda_i(G(\alpha_k))| \leq 2(\alpha - \alpha_k) (\sigma_1(X_1) + \sigma_1(X_2))^2 \leq \frac{2}{K} (\sigma_1(X_1) + \sigma_1(X_2))^2 ,
\]

\[
|\lambda_i(G(\alpha)) - \lambda_i(G(\alpha_{k+1}))| \leq 2(\alpha_{k+1} - \alpha) (\sigma_1(X_1) + \sigma_1(X_2))^2 \leq \frac{2}{K} (\sigma_1(X_1) + \sigma_1(X_2))^2 . \tag{1}
\]

**Proof.** Using the singular value decomposition of \( X(\alpha) = U(\alpha) \Sigma(\alpha) V^\top(\alpha) \) (being \( U(\alpha) \in \mathbb{R}^{m \times m} \) and \( V(\alpha) \in \mathbb{R}^{n \times n} \) orthogonal matrices, and \( \Sigma(\alpha) \in \mathbb{R}^{m \times n} \) a rectangular matrix whose \( q = \min\{m, n\} \) elements on its main diagonal are the singular values \( \sigma_i(X(\alpha)) \)), ordered from the largest singular value to the smallest one, one gets

\[
G(\alpha) = X(\alpha)X^\top(\alpha) = U(\alpha) \Sigma(\alpha) V^\top(\alpha) (U(\alpha) \Sigma(\alpha) V^\top(\alpha))^\top,
\]

\[
= U(\alpha) \Sigma(\alpha) V^\top(\alpha) \Sigma^\top(\alpha) V(\alpha) = U(\alpha) \Lambda(\alpha) U^\top(\alpha), \tag{2}
\]

where, denoting by \( I_{n \times n} \in \mathbb{R}^{n \times n} \) the identity matrix, the property \( V^\top(\alpha) V(\alpha) = I_{n \times n} \) has been used, and \( \Lambda(\alpha) \triangleq \Sigma(\alpha) \Sigma^\top(\alpha) \in \mathbb{R}^{m \times m} \) is a diagonal matrix whose elements on its main diagonal are the squares \( \sigma_i^2(X(\alpha)) \) of the singular values \( \sigma_i(X(\alpha)) \) of \( X(\alpha) \), plus \( m - n \) additional zeros (if and only if \( m > n \)). The \( \sigma_i^2(X(\alpha)) \) and the possible \( m - n \) additional zeros are also the eigenvalues \( \lambda_i(G(\alpha)) \) of \( G(\alpha) \), since this is a symmetric and positive semi-definite matrix. We consider first the case \( m \leq n \), then the case \( m > n \).

*Case 1. \( m \leq n \).* We exploit the matrix perturbation bound on singular values provided in [10, Theorem 3.3.16 (c)], according to which, given any two matrices \( A, B \in \mathbb{R}^{m \times n} \), one has, for all \( i = 1, \ldots, \min\{m, n\} = m \),

\[
|\sigma_i(A) - \sigma_i(A + B)| \leq \sigma_i(B) . \tag{3}
\]

Denoting by \( \Delta \alpha \) a variation of \( \alpha \), we apply Eq. (3) with \( A = X(\alpha) \) and \( B = X(\alpha + \Delta \alpha) - X(\alpha) = \Delta \alpha (X_1 - X_2) \). Recalling the relation \( \lambda_i(G(\alpha)) = \sigma_i^2(X(\alpha)) \) valid for all \( i = 1, \ldots, m \), and the fact that \( \sigma_i(X(\alpha)) \geq 0 \), we get

\[
|\lambda_i(G(\alpha + \Delta \alpha)) - \lambda_i(G(\alpha))| = |\sigma_i^2(X(\alpha + \Delta \alpha)) - \sigma_i^2(X(\alpha))|
\]
by PCA applied to the data matrices

Definition. Let the formal definition of Jordan canonical angles (see also [20, 22]),

being the bases chosen to minimize such angles. Before stating the bound, we recall

between corresponding elements of the orthonormal bases of the two subspaces,
different values of \( \alpha \)
d\ref{ref}{andrea bacigalupo} refers to the Jordan canonical angles between two

cases, considered, as its orthonormal eigenvectors are the principal directions. The bound

Lipschitz continuity of the eigenvalues of \( G \)

Remark 1. The bounds expressed by Eqs. (1a) and (1b), whose proofs show the

The proof is the same as above for all but the last (smallest) \( m-n \) eigenvalues of \( G(\alpha) \) and \( G(\alpha_k) \). However, the latter eigenvalues are all equal to 0, and the bound (1a) still holds trivially for them.

Finally, the proof of Eq. (1b) is similar to the one of Eq. (1a) reported

above.

\( \square \)

Case 2. \( m > n \). The proof is the same as above for all but the last (smallest) \( m-n \) eigenvalues of \( G(\alpha) \) and \( G(\alpha_k) \). However, the latter eigenvalues are all equal to 0, and the bound (1a) still holds trivially for them.

Finally, the proof of Eq. (1b) is similar to the one of Eq. (1a) reported

above.

Matrix perturbation bound on the set of invariant subspaces found
by PCA in the case of a convex combination of two data matrices. In
this section, a perturbation bound on the set of invariant subspaces found by PCA
is provided, for the same case considered in Section 3. In the present analysis,
however, instead of the Gram matrix \( G = XX^\top \), the PCA matrix \( C = \frac{1}{m} X^\top X \) is
considered, as its orthonormal eigenvectors are the principal directions. The bound
refers to the Jordan canonical angles between two \( d \)-dimensional subspaces found
by PCA applied to the data matrices \( X(\alpha) \) generated from \( X_1 \) and \( X_2 \) for two
different values of \( \alpha \in [0, 1] \). These, loosely speaking, represent the smallest angles
between corresponding elements of the orthonormal bases of the two subspaces,
being the bases chosen to minimize such angles. Before stating the bound, we recall
the formal definition of Jordan canonical angles (see also [20, 22]).

Definition. Let \( E, F \subseteq \mathbb{R}^n \) be two \( d \)-dimensional subspaces of \( \mathbb{R}^n \) \( (1 \leq d \leq n) \), and
\( E, F \in \mathbb{R}^{n \times d} \) be two matrices with orthonormal columns such that \( \text{range}(E) = E \)
and \( \text{range}(F) = F \). Then, the first Jordan canonical angle between \( E \) and \( F \) is

\[
\theta_1(E, F) = \max_{x \in E} \max_{y \in F} \arccos(x^\top y) = \arccos(x_1^\top y_1),
\]

where \( \| \cdot \|_2 \) denotes the Euclidean norm, and the column vectors \( x_1 \in E \) and
\( y_1 \in F \) are the maximizers of the objective function reported in Eq. (6). Similarly,
for $k = 2, \ldots, d$, the $k$-th Jordan canonical angle between $\mathcal{E}$ and $\mathcal{F}$ is

$$\theta_k(\mathcal{E}, \mathcal{F}) \equiv \max_{x \in \mathcal{E}, \|x\|_2 = 1} \max_{y \in \mathcal{F}, \|y\|_2 = 1} \arccos(x^\top y) = \arccos(x_k^\top y_k),$$

(7)

where the column vectors $x_k \in \mathcal{E}$ and $y_k \in \mathcal{F}$ are the maximizers of the objective function reported in Eq. (7).

By construction, the $x_k$ and the $y_k$ form orthonormal bases of $\mathcal{E}$ and $\mathcal{F}$, respectively. Indeed, it follows from the construction above that each $x_k$ has unit norm and, for $k = 2, \ldots, d$, it is orthogonal to all its preceding $x_{k'}$ ($k' = 1, \ldots, k-1$). Similarly, each $y_k$ has unit norm and, for $k = 2, \ldots, d$, it is orthogonal to all its preceding $y_{k'}$ ($k' = 1, \ldots, k-1$). It can be also proved (see, e.g., [16]) that the Jordan canonical angles can be written in the alternative form

$$\theta_k(\mathcal{E}, \mathcal{F}) = \arccos(\sigma_k(E^\top F)), \; k = 1, \ldots, d,$$

(8)

being $\sigma_k(E^\top F)$ the $k$-th singular value of the matrix $E^\top F$. The Jordan canonical angles $\theta_k(\mathcal{E}, \mathcal{F})$ ($k = 1, \ldots, d$) form the vector $\theta \in \mathbb{R}^d$. In the following, the vector $\sin(\theta(\mathcal{E}, \mathcal{F})) \in \mathbb{R}^d$ (whose elements are $\sin(\theta_k(\mathcal{E}, \mathcal{F}))$, for $k = 1, \ldots, d$) is also considered. It readily follows from their definitions that $0 \leq \theta_k(\mathcal{E}, \mathcal{F}) \leq \theta_2(\mathcal{E}, \mathcal{F}) \leq \cdots \leq \theta_d(\mathcal{E}, \mathcal{F}) \leq \pi/2$.

In order to state the next proposition, the following notation is introduced (with a few repetitions from Section 2). Let $X_1, X_2 \in \mathbb{R}^{m \times n}$ be two data matrices, $\alpha \in [0, 1]$, $C(\alpha) \equiv \frac{1}{m}X_1^\top (\alpha)X(\alpha) \in \mathbb{R}^{n \times n}$ be the PCA matrix of their convex combination $X(\alpha) \equiv \alpha X_1 + (1 - \alpha) X_2$ with weights $\alpha$ and $1 - \alpha$, $K \in \mathbb{N}$ and, for $k = 0, 1, \ldots, K$, $\alpha_k \equiv \frac{k}{K}$. Let the non-negative eigenvalues of $C(\alpha)$ and $C(\alpha_k)$ be ordered non-increasingly, respectively, as $\lambda_1(C(\alpha)) \geq \lambda_2(C(\alpha)) \geq \cdots \geq \lambda_n(C(\alpha))$ and $\lambda_1(C(\alpha_k)) \geq \lambda_2(C(\alpha_k)) \geq \cdots \geq \lambda_n(C(\alpha_k))$, and let $\{e_1(C(\alpha)), e_2(C(\alpha)), \ldots, e_n(C(\alpha))\}$ and $\{e_1(C(\alpha_k)), e_2(C(\alpha_k)), \ldots, e_n(C(\alpha_k))\}$ be two corresponding bases of orthonormal eigenvectors of $C(\alpha)$ and $C(\alpha_k)$, respectively. For $1 \leq r \leq s \leq n$, let $\mathcal{E}^{r-s}(\alpha), \mathcal{F}^{r-s}(\alpha) \subseteq \mathbb{R}^n$ be the two $(s - r + 1)$-dimensional subspaces of $\mathbb{R}^n$ generated by $e_r(C(\alpha)), e_{r+1}(C(\alpha)), \ldots, e_s(C(\alpha))$ and $e_r(C(\alpha_k)), e_{r+1}(C(\alpha_k)), \ldots, e_s(C(\alpha_k))$, respectively (these two subspaces are invariant with reference to the application of $C(\alpha)$ and $C(\alpha_k)$, respectively). Moreover, likewise in Section 2, let $\sigma_1(X(\alpha))$ and $\sigma_1(X(\alpha_k))$ be the largest singular values of $X(\alpha)$ and $X(\alpha_k)$, respectively. Finally, let the so-called eigengap $\delta_1(\mathcal{E}^{r-s}(\alpha), \mathcal{F}^{r-s}(\alpha_k))$ be defined as

$$\delta_1(\mathcal{E}^{r-s}(\alpha), \mathcal{F}^{r-s}(\alpha_k)) \equiv \inf\{|\lambda - \hat{\lambda}| : \lambda \in [\lambda_s(C(\alpha_k)), \lambda_r(C(\alpha_k))],$$

$$\hat{\lambda} \in (-\infty, \lambda_{s+1}(C(\alpha)) \cup [\lambda_{r-1}(C(\alpha)), +\infty)), (9)$$

assuming by convention $\lambda_0(C(\alpha)) \equiv +\infty$, $\lambda_{n+1}(C(\alpha)) \equiv -\infty$, and let its approximation $\delta_2(\alpha, \mathcal{E}^{r-s}(\alpha_k))$ be defined as

$$\delta_2(\alpha, \mathcal{E}^{r-s}(\alpha_k)) \equiv \inf\{|\lambda - \hat{\lambda}| : \lambda \in [\lambda_s(C(\alpha_k)), \lambda_r(C(\alpha_k))],$$

$$\hat{\lambda} \in (-\infty, \lambda_{s+1}(C(\alpha_k)) + \frac{2|\alpha - \alpha_k|}{m} (\sigma_1(X_1) + \sigma_1(X_2))^2 + [\lambda_{r-1}(C(\alpha_k)) - \frac{2|\alpha - \alpha_k|}{m} (\sigma_1(X_1) + \sigma_1(X_2))^2, +\infty)), (10)$$

assuming by convention $\lambda_0(C(\alpha)) \equiv +\infty$, $\lambda_{n+1}(C(\alpha)) \equiv -\infty$, and let its approximation $\delta_2(\alpha, \mathcal{E}^{r-s}(\alpha_k))$ be defined as

$$\delta_2(\alpha, \mathcal{E}^{r-s}(\alpha_k)) \equiv \inf\{|\lambda - \hat{\lambda}| : \lambda \in [\lambda_s(C(\alpha_k)), \lambda_r(C(\alpha_k))],$$

$$\hat{\lambda} \in (-\infty, \lambda_{s+1}(C(\alpha_k)) + \frac{2|\alpha - \alpha_k|}{m} (\sigma_1(X_1) + \sigma_1(X_2))^2 + [\lambda_{r-1}(C(\alpha_k)) - \frac{2|\alpha - \alpha_k|}{m} (\sigma_1(X_1) + \sigma_1(X_2))^2, +\infty)). (10)$$
Loosely speaking, the eigengap \( \delta_1(\mathcal{E}^{r,s}(\alpha), \mathcal{F}^{r,s}(\alpha_k)) \) measures the distance between the set of eigenvalues associated with a suitable subset of eigenvectors of \( C(\alpha_k) \), and the set of eigenvalues associated with another suitable subset of eigenvectors of \( C(\alpha) \), whereas its approximation \( \delta_2(\alpha, \mathcal{F}^{r,s}(\alpha_k)) \) is inspired by Proposition 1.

**Proposition 2.** For any \( k = 0, 1, \ldots, K-1, \alpha \in [\alpha_k, \alpha_{k+1}] \), and \( 1 \leq r \leq s \leq n \), and in the common case in which the quantities \( \delta_1(\mathcal{E}^{r,s}(\alpha), \mathcal{F}^{r,s}(\alpha_k)), \delta_2(\alpha, \mathcal{F}^{r,s}(\alpha_k)), \delta_1(\mathcal{E}^{r,s}(\alpha), \mathcal{F}^{r,s}(\alpha_{k+1})), \delta_2(\alpha, \mathcal{F}^{r,s}(\alpha_{k+1})) \) are larger than zero, the following holds:

\[
\sqrt{s-r+1} \sin(\theta_1(\mathcal{E}^{r,s}(\alpha), \mathcal{F}^{r,s}(\alpha))) \
\leq \frac{\|C(\alpha) - C(\alpha_k)\|_F}{\delta_1(\mathcal{E}^{r,s}(\alpha), \mathcal{F}^{r,s}(\alpha_k))} \
\leq \frac{\|C(\alpha) - C(\alpha_k)\|_F}{\delta_2(\alpha, \mathcal{F}^{r,s}(\alpha_k))} \
\leq \frac{\alpha - \alpha_k}{m} \|X_1 - X_2\|^\top X(\alpha_k)(X_1 - X_2)\|_F + \frac{\alpha - \alpha_k}{m} \|X_1 - X_2\|^\top(X_1 - X_2)\|_F \\
\leq \frac{1}{2\alpha - \alpha_k} \|X_1 - X_2\|^\top X(\alpha_k)(X_1 - X_2)\|_F + \frac{1}{\delta_2(\alpha, \mathcal{F}^{r,s}(\alpha_k))} \|X_1 - X_2\|^\top(X_1 - X_2)\|_F,
\]

where \( \| \cdot \|_F \) denotes the Frobenius norm.

**Proof.** The first inequality

\[
\sqrt{s-r+1} \sin(\theta_1(\mathcal{E}^{r,s}(\alpha), \mathcal{F}^{r,s}(\alpha_k))) \leq \|\sin(\theta(\mathcal{E}^{r,s}(\alpha), \mathcal{F}^{r,s}(\alpha_k)))\|_2,
\]

is obtained directly from the definition of \( \theta(\mathcal{E}^{r,s}(\alpha), \mathcal{F}^{r,s}(\alpha_k)) \) and the property \( 0 \leq \theta_1(\mathcal{E}, \mathcal{F}) \leq \theta_2(\mathcal{E}, \mathcal{F}) \leq \ldots \leq \theta_d(\mathcal{E}, \mathcal{F}) \leq \frac{\pi}{2} \). The second inequality

\[
\|\sin(\theta(\mathcal{E}^{r,s}(\alpha), \mathcal{F}^{r,s}(\alpha_k)))\|_2 \leq \frac{\|C(\alpha) - C(\alpha_k)\|_F}{\delta_1(\mathcal{E}^{r,s}(\alpha), \mathcal{F}^{r,s}(\alpha_k))},
\]

is a direct application of the simplified version\(^2\) from [21, Theorem 1] of the well-known Davis-Kahan theorem in matrix perturbation theory [16, Theorem V.3.6]. The third inequality

\[
\frac{\|C(\alpha) - C(\alpha_k)\|_F}{\delta_1(\mathcal{E}^{r,s}(\alpha), \mathcal{F}^{r,s}(\alpha_k))} \leq \frac{\|C(\alpha) - C(\alpha_k)\|_F}{\delta_2(\alpha, \mathcal{F}^{r,s}(\alpha_k))},
\]

\(^2\)In the sense that the bound from [21, Theorem 1] is looser than the one in [16, Theorem V.3.6], but it is also easier to apply.
comes from $0 \leq \delta_2(\alpha, \mathcal{F}^r, \mathcal{F}^s)(\alpha_k)) \leq \delta_1(\mathcal{E}^r, \mathcal{F}^s)(\alpha_k)$ (which follows from Eq. (1a) in Proposition 1 and the fact that, when $\lambda_i(C(a))$ is positive, then one has $\lambda_i(C(a)) = \frac{1}{m}\lambda_i(G(a))$, otherwise $\lambda_i(C(a)) = 0$). Finally, the last inequalities

$$
\frac{\|C(a) - C(\alpha_k)\|_F}{\delta_2(\alpha, \mathcal{F}^r, \mathcal{F}^s)(\alpha_k))} \\
\leq \frac{\alpha - \alpha_k}{m} \|X_1 - X_2\|_{\mathcal{F}(\alpha_k)} + X^T(\alpha_k)(X_1 - X_2)\|_F + \frac{(\alpha - \alpha_k)^2}{m} \|X_1 - X_2\|_{\mathcal{F}(\alpha_k)}
$$

$$
\leq \frac{1}{Km} \|X_1 - X_2\|_{\mathcal{F}(\alpha_k)} + X^T(\alpha_k)(X_1 - X_2)\|_F + \frac{1}{K^2m} \|X_1 - X_2\|_{\mathcal{F}(\alpha_k)}
$$

come from bounding from above the term $\|C(a) - C(\alpha_k)\|_F$ as follows (using the triangle inequality for matrix norms and recalling that $0 \leq \alpha - \alpha_k \leq \frac{1}{K}$):

$$
\|C(a) - C(\alpha_k)\|_F = \left\| \frac{1}{m} X^T(a)X(a) - \frac{1}{m} X^T(\alpha_k)X(\alpha_k) \right\|_F
$$

$$
= \left\| \frac{1}{m} X^T(\alpha_k + \alpha - \alpha_k)X(\alpha_k + \alpha - \alpha_k) - \frac{1}{m} X^T(\alpha_k)X(\alpha_k) \right\|_F
$$

$$
= \frac{1}{m} \left\| X^T(\alpha_k)X(\alpha_k) + (\alpha - \alpha_k) \left[ (X_1 - X_2)^T X(\alpha_k) + X^T(\alpha_k)(X_1 - X_2) \right] + (\alpha - \alpha_k)^2 (X_1 - X_2)^T (X_1 - X_2) - X^T(\alpha_k)X(\alpha_k) \right\|_F
$$

$$
= \frac{1}{m} \left\| (\alpha - \alpha_k) \left[ (X_1 - X_2)^T X(\alpha_k) + X^T(\alpha_k)(X_1 - X_2) \right] + (\alpha - \alpha_k)^2 (X_1 - X_2)^T (X_1 - X_2) \right\|_F
$$

$$
\leq \frac{\alpha - \alpha_k}{m} \|X_1 - X_2\|_{\mathcal{F}(\alpha_k)} + X^T(\alpha_k)(X_1 - X_2)\|_F + \frac{(\alpha - \alpha_k)^2}{m} \|X_1 - X_2\|_{\mathcal{F}(\alpha_k)}
$$

$$
\leq \frac{1}{Km} \|X_1 - X_2\|_{\mathcal{F}(\alpha_k)} + X^T(\alpha_k)(X_1 - X_2)\|_F + \frac{1}{K^2m} \|X_1 - X_2\|_{\mathcal{F}(\alpha_k)}
$$

Finally, the proof of Eq. (11b) is similar to the one of Eq. (11a) reported above.

**Remark 2.** The bound provided by Eq. (11a) can be applied only in the case in which the quantities $\delta_1(\mathcal{E}^r, \mathcal{F}^s)(\alpha_k))$ and $\delta_2(\alpha, \mathcal{F}^r, \mathcal{F}^s)(\alpha_k))$ are larger than zero. This holds surely when all the following conditions are satisfied:

a. $\lambda_{r-1}(C(\alpha_k)) \neq \lambda_r(C(\alpha_k))$;

b. $\lambda_{s+1}(C(\alpha_k)) \neq \lambda_s(C(\alpha_k))$;

c. $\alpha - \alpha_k$ is small enough.

A similar comment holds for the bound provided by Eq. (11b). Moreover, the proof of Proposition 2 shows that the directions of the eigenvectors of $C(\alpha)$ depend in a Lipschitz-continuous way on $\alpha$, in all the intervals in which either conditions a)-c) above or the analogous ones for Eq. (11b) hold.

**Remark 3.** A particularly interesting case in Proposition 2 is when $r = s$; in this situation, $\mathcal{E}^r, \mathcal{F}^r, \mathcal{F}^s(\alpha_k)$ and $\mathcal{F}^{r,s}(\alpha_k+1)$ are the 1-dimensional subspaces generated, respectively, by the $r$-th principal direction $e_r(C(\alpha))$ of $C(\alpha)$, the $r$-th principal direction $e(C(\alpha_k))$ of $C(\alpha_k)$, and the $r$-th principal direction $e(C(\alpha_k+1))$ of $C(\alpha_k+1)$.
Likewise Eqs. (1a) and (1b), Eqs. (11a) and (11b) can be used in the following way. First, one finds the sets of eigenvectors of the matrices $C(\alpha_k)$, for $k = 1, \ldots, K$. Second, for each $\alpha \in [0, 1]$, one finds the associated $\alpha_0$ and $\alpha_{k+1}$, then applies Eqs. (11a) and (11b) to locate approximately the directions of the orthonormal eigenvectors of the new matrix $C(\alpha)$. In particular, for all $i = 1, \ldots, m$, one chooses the best among the bounds provided by Eqs. (11a) and (11b): e.g., for the case $r = s = i$, the smallest between the upper bound on $\sin(\theta_1(E^{i,i}(\alpha), F^{i,i}(\alpha_k)))$ from Eq. (11a) and the upper bound on $\sin(\theta_1(E^{i,i}(\alpha), F^{i,i}(\alpha_{k+1})))$ from Eq. (11b), as done in the numerical example reported later in Section 4.

Remark 5. A result similar to Proposition 2 can be obtained by replacing the PCA matrices $C(\alpha)$ and $C(\alpha_k)$ with the Gram matrices $G(\alpha)$ and $G(\alpha_k)$, respectively. However, it would be of less direct application than Proposition 2, since one is usually interested in the principal directions, which are obtained as suitable orthonormal eigenvectors of the PCA matrices (when they are associated with their $d$ largest positive eigenvalues). Nevertheless, the eigenvectors of the PCA and Gram matrices associated with positive eigenvalues are related, in the sense that, given one such eigenvector for one of the two matrices, one can construct (and associate with the former) an eigenvector of the other matrix, which is also associated with a positive eigenvalue$^3$. In this way, a matrix perturbation bound on the directions of the eigenvectors of two Gram matrices associated with positive eigenvalues could be translated into a matrix perturbation bound on the directions of the corresponding eigenvectors of the two related PCA matrices.

4. Numerical results. As a simple example of application of Propositions 1 and 2, we set $m = 10$, $n = 5$, and consider the two following artificially-generated data matrices $X_1, X_2 \in \mathbb{R}^{10 \times 5}$:

$$
X_1 = \begin{bmatrix}
+1 & +1 & -1 & +1 & -1 \\
-1 & +1 & +1 & -1 & +1 \\
-1 & +1 & +1 & +1 & -1 \\
+1 & -1 & +1 & -1 & -1 \\
+1 & -1 & -1 & +1 & +1 \\
+1 & -1 & -1 & -1 & +1 \\
+1 & +1 & -1 & -1 & +1 \\
+1 & +1 & +1 & -1 & +1 \\
+1 & +1 & +1 & +1 & +1 \\
\end{bmatrix}, \quad X_2 = \begin{bmatrix}
-1 & +1 & -1 & -1 & -1 \\
-1 & -1 & -1 & +1 & -1 \\
-1 & -1 & +1 & -1 & +1 \\
-1 & +1 & +1 & -1 & +1 \\
-1 & +1 & +1 & -1 & +1 \\
-1 & -1 & -1 & -1 & +1 \\
-1 & +1 & -1 & -1 & +1 \\
+1 & +1 & -1 & -1 & -1 \\
+1 & +1 & +1 & -1 & -1 \\
+1 & +1 & +1 & -1 & -1 \\
\end{bmatrix}.
$$

Then, in Fig. 1 (a), we report, as functions of $\alpha \in [0, 1]$, the (numerically evaluated) positive eigenvalues $\lambda_1(G(\alpha)), \ldots, \lambda_5(G(\alpha))$ of the Gram matrix $G(\alpha)$ associated with the data matrix $X(\alpha) = \alpha X_1 + (1 - \alpha)X_2$, together with their best lower bounds derived from the first inequalities in Eqs. (1a) and (1b) in Proposition 1 with $K = 50$, and their best upper bounds derived from the same inequalities, still with $K = 50$. Similarly, in Fig. 1 (b), we report, for $K = 50$, $i = 1$, and each

$^3$Indeed, if $u \in \mathbb{R}^n$ is an eigenvector of $XX^T$ associated with a positive eigenvalue $\lambda$, then $X^T u \neq 0_n$, where $0_n \in \mathbb{R}^n$ denotes the column vector made of $n$ zeros (because $XX^T u = \lambda u \neq 0_n$ by the assumptions on $u$). Hence, $v = X^T u \in \mathbb{R}^n$ is an eigenvector of $\frac{1}{m} X^T X$ associated with the positive eigenvalue $\frac{\lambda}{m}$. Moreover, $u = \frac{1}{\sqrt{m}} X v$. Similarly, starting from an eigenvector $v \in \mathbb{R}^n$ of $\frac{1}{m} X^T X$ associated with a positive eigenvalue of that matrix, one can construct a corresponding eigenvector $u \in \mathbb{R}^m$ of $XX^T$ associated with a positive eigenvalue of the latter matrix.
A case of convex combination of two data matrices: sampled gradient-fields in multi-objective optimization problems. The theoretical framework considered in Sections 2 and 3 has application, e.g., in the combination of PCA with the so-called weighted sum method, which is used in the context of multi-objective optimization [6]. In the case of two objective functions, this method approximates the Pareto frontier of a multi-objective optimization problem by maximizing, with

\[ \sin(\theta_{1,\text{min}}(\alpha)) = \min\{\sin(\theta_1(E^{i,i}(\alpha), F^{i,i}(\alpha_k))), \sin(\theta_1(E^{i,i}(\alpha), F^{i,i}(\alpha_{k+1}))\}, \]

and the smallest upper bound on it, based on the second to last inequalities in Eqs. (11a) and (11b) in Proposition 2 (only the case \( i = 1 \) is shown in the figure, to avoid overlaps with the similar curves obtained for \( i = 2, \ldots, 5 \)). It is worth observing that the sawtooth functional shape of the ground truth in Fig. 1 (b) is due to the fact that \( \alpha_k \) and \( \alpha_{k+1} \) vary discontinuously with \( \alpha \).

\( \alpha \in [0, 1] \), the (numerically evaluated) smallest between \( \sin(\theta_1(E^{i,i}(\alpha), F^{i,i}(\alpha_k))) \) and \( \sin(\theta_1(E^{i,i}(\alpha), F^{i,i}(\alpha_{k+1}))) \), i.e.

\[ \sin(\theta_{1,\text{min}}(\alpha)) = \min\{\sin(\theta_1(E^{i,i}(\alpha), F^{i,i}(\alpha_k))), \sin(\theta_1(E^{i,i}(\alpha), F^{i,i}(\alpha_{k+1}))\}, \]

5. A case of convex combination of two data matrices: sampled gradient-fields in multi-objective optimization problems. The theoretical framework considered in Sections 2 and 3 has application, e.g., in the combination of PCA with the so-called weighted sum method, which is used in the context of multi-objective optimization [6]. In the case of two objective functions, this method approximates the Pareto frontier of a multi-objective optimization problem by maximizing, with

\[ \text{Or minimizing, depending on the specific context of application.} \]
respect to the column vector $p \in P \subseteq \mathbb{R}^n$, the trade-off

$$J_\alpha(p) \doteq \alpha J_1(p) + (1 - \alpha) J_2(p), \quad (19)$$

between the two objective functions $J_1(p)$ and $J_2(p)$, for different values of the parameter $\alpha \in [0, 1]$ (an adaptive version of the method can be applied in cases for which the classical weighted sum method fails, e.g., when the Pareto frontier is nonconcave\(^5\) [12]). Assuming that both $J_1(p)$ and $J_2(p)$ are differentiable and the optimization problem is unconstrained (i.e., $P = \mathbb{R}^n$) or that it can be reduced to an unconstrained optimization problem by using a suitable penalization approach, one could perform the optimization numerically by applying, e.g., the classical gradient method, possibly combined with a multi-start approach. In order to reduce the computational effort needed for the exact computation of the gradient at each iteration of the gradient method, one could replace it with its approximate obtained by applying PCA to the gradient field $\nabla J_\alpha(p)$ evaluated on a subset of points $p_j \in P$ (for $j = 1, \ldots, m$), then projecting the exact gradient onto the subspace generated by the average of the gradients $\nabla J_\alpha(p_j)$, and by the first principal directions found by PCA, when this is applied to the dataset $\{\nabla J_\alpha(p_j)\}_{j=1}^m$, after a pre-processing step, which makes it centered\(^6\). Due to the structure of the objective function $J_\alpha(p)$, such dataset (represented by a data matrix $X_\alpha$) would be made of the convex combination (with coefficients $\alpha$ and $1 - \alpha$) of the two datasets $\{\nabla J_1(p_j)\}_{j=1}^m$ and $\{\nabla J_2(p_j)\}_{j=1}^m$, represented respectively by the two data matrices $X_1$ and $X_2$ (a similar comment holds for the centered version of the dataset). In this context, the results of our theoretical analysis reported in Section 2 could be useful to restrict the application of the weighted sum method to a coarse grid of values $\alpha_k$ for $\alpha \in [0, 1]$, from which one could infer, for other values of $\alpha$, the empirical variances of the projections of the (de-meaned) data matrices $X^{(c)}(\alpha)$ onto the principal directions either selected or discarded by PCA, when PCA is applied to each such data matrix $X^{(c)}(\alpha)$. Similarly, the results of our theoretical analysis reported in Section 3 could be useful to investigate how the principal directions themselves change by varying the parameter $\alpha$.

5.1. The case of unconstrained multi-objective maximization with quadratic and concave objective functions. In this subsection, we consider the following example of an unconstrained multi-objective maximization problem with quadratic and concave objective functions, in order to investigate theoretically how PCA can be applied to this simple case, combined, e.g., with a suitable multi-start optimization algorithm. In this subsection, the two objective functions $J_1 : \mathbb{R}^n \to \mathbb{R}$ and $J_2 : \mathbb{R}^n \to \mathbb{R}$ are defined as

$$J_1(p) \doteq -\frac{1}{2} p^\top Q_1 p + v_1^\top p, \quad (20)$$

and

$$J_2(p) \doteq -\frac{1}{2} p^\top Q_2 p + v_2^\top p, \quad (21)$$

\(^5\)Respectively, nonconvex in the case of a multi-objective minimization problem.

\(^6\)It is common practice to apply PCA to centered (also called de-meaned) data matrices $X^{(c)}$, i.e., having the form $X^{(c)} \doteq X - 1_m x^\top$, where $1_m \in \mathbb{R}^m$ denotes a column vector made of $m$ ones, and $x \in \mathbb{R}^n$ is a column vector whose elements are the averages of the corresponding columns of $X$. This does not change the quality of the results of the theoretical analysis, because, by linearity, the centered convex combination of two data matrices $X_1$ and $X_2$ is equal to the convex combination of the two respective centered data matrices $X_1^{(c)}$ and $X_2^{(c)}$. 
being $Q_1, Q_2 \in \mathbb{R}^{n \times n}$ two given symmetric and positive definite matrices, and $v_1, v_2 \in \mathbb{R}^n$ two given column vectors. For each $\alpha \in [0, 1]$, no constraints are present in the maximization of $J_\alpha(p) = \alpha J_1(p) + (1 - \alpha)J_2(p)$. For each $\alpha \in [0, 1]$, let
\[ Q(\alpha) = \alpha Q_1 + (1 - \alpha)Q_2, \tag{22} \]
and
\[ v(\alpha) = \alpha v_1 + (1 - \alpha)v_2. \tag{23} \]
Then, since $Q(\alpha)$ is symmetric and positive definite, the unique optimal solution to the optimization problem
\[ \max_{p \in \mathbb{R}^n} J_\alpha(p), \tag{24} \]
is
\[ p_\alpha^* = Q^{-1}(\alpha)v(\alpha), \tag{25} \]
and the corresponding optimal objective value is
\[ J_\alpha^* = J_\alpha(p_\alpha^*) = \frac{1}{2}v^T(\alpha)Q^{-1}(\alpha)v(\alpha). \tag{26} \]
Moreover, the gradient of the objective function $J_\alpha(p)$ is
\[ \nabla J_\alpha(p) = \alpha \nabla J_1(p) + (1 - \alpha)\nabla J_2(p) \]
\[ = -(\alpha Q_1 + (1 - \alpha)Q_2)p + \alpha v_1 + (1 - \alpha)v_2 \]
\[ = -Q(\alpha)p + v(\alpha). \tag{27} \]
We divide the analysis in the following steps:
1) Let us compute the gradient $\nabla J_\alpha(p)$ on a set of $m$ training examples $p_j$ ($j = 1, \ldots, m$), where the $p_j$ are independent and identically distributed random vectors with zero mean, and have the common covariance matrix $E\{p_jp_j^\top\} = I_{n \times n}$, where $E$ denotes the expectation operator. Then, the mean of the gradient $\nabla J_\alpha(p_j)$ is
\[ E\{\nabla J_\alpha(p_j)\} = -Q(\alpha)E\{p_j\} + v(\alpha) = -Q(\alpha)0_n + v(\alpha) = v(\alpha), \tag{28} \]
whereas its covariance matrix is
\[ E\{(\nabla J_\alpha(p_j) - E\{\nabla J_\alpha(p_j)\})(\nabla J_\alpha(p_j) - E\{\nabla J_\alpha(p_j)\})^\top\} \]
\[ = E\{(-Q(\alpha)p_j)(-Q(\alpha)p_j)^\top\} \]
\[ = E\{Q(\alpha)p_jp_j^\top Q^\top(\alpha)\} \]
\[ = Q(\alpha)I_{n \times n}Q^\top(\alpha) \]
\[ = Q^2(\alpha), \tag{29} \]
being $Q(\alpha)$ symmetric. If $m$ is large enough and mild assumptions are made (e.g., all the moments of the random vector $p_j$ up to the order 4 are finite), with high probability the PCA matrix $C^{(\alpha)} = \frac{1}{m}X^{(\alpha)}(\alpha)(X^{(\alpha)}(\alpha))^\top$ is approximately equal to this covariance matrix (by Chebyshev’s weak law of large numbers [14, Section 13.4.2]), having denoted by $X^{(\alpha)}$ the centered version of the data matrix $X(\alpha) = \alpha X_1 + (1 - \alpha)X_2$, where the $j$-th row of the matrix $X_j \in \mathbb{R}^{m \times n}$ is $(\nabla J_1(p_j))^\top$, and the $j$-th row of the matrix $X_2 \in \mathbb{R}^{m \times n}$ is $(\nabla J_2(p_j))^\top$.
2) The matrices $Q(\alpha)$ and $Q^2(\alpha)$ have the same eigenspaces, and their eigenvalues are ordered in the same way. Moreover, by making the approximation $C^{(\alpha)} \simeq Q^2(\alpha)$, the first $d < n$ principal directions $e_i(C^{(\alpha)}(\alpha))$ of the PCA matrix $C^{(\alpha)}(\alpha)$ ($i = 1, \ldots, d$) are also eigenvectors of $Q(\alpha)$ associated with its $d$
3) Let \( P(α) = \sum_{i=1}^{d} e_i (C^{(α)}(α)) Q(α) e_i (C^{(α)}(α)) \) be the orthogonal projection matrix onto the subspace of \( \mathbb{R}^n \) generated by the first \( d \) principal directions. Then, by decomposing the vector of optimization variables as
\[
p = P(α)p + (I_{n \times n} - P(α))p = p_{α,∥} + p_{α,⊥},
\]
we can express the objective function \( J_α(p) \) as follows:
\[
J_α(p) = -\frac{1}{2}(p_{α,∥} + p_{α,⊥})^T Q(α)(p_{α,∥} + p_{α,⊥}) + v^T(α)(p_{α,∥} + p_{α,⊥}),
\]
\[
= \left[ -\frac{1}{2}p_{α,∥}^T Q(α)p_{α,∥} + v^T(α)p_{α,∥} \right] + \left[ -\frac{1}{2}p_{α,⊥}^T Q(α)p_{α,⊥} + v^T(α)p_{α,⊥} \right];
\]
(31)

4) The two vectors of optimization variables \( p_{α,∥} \) and \( p_{α,⊥} \) can be optimized independently. Hence, the optimal solution \( p^o_α \) can be also written as
\[
p^o_α = p^o_{α,∥} + p^o_{α,⊥},
\]
(32)
and the associated optimal objective value can be also written as
\[
J^o_α = \left[ -\frac{1}{2}(p^o_{α,∥})^T Q(α)p^o_{α,∥} + v^T(α)p^o_{α,∥} \right] + \left[ -\frac{1}{2}(p^o_{α,⊥})^T Q(α)p^o_{α,⊥} + v^T(α)p^o_{α,⊥} \right];
\]
(33)

5) Let \( p^{(0)} \) be a random initial choice for \( p \), generated likewise the training examples \( p_j \). If one maximizes \( J_α(p) \) with respect to \( p_{α,∥} \) alone (e.g., by imposing the first-order optimality condition for unconstrained maximization in the first term of the expression (31) of \( J_α(p) \), or by moving according to a gradient-based optimization algorithm along an affine subspace parallel to the subspace generated by the first \( d \) principal directions of the PCA matrix \( C^{(α)}(α) \)), one can find the optimal \( p^o_{α,∥} \). However, by doing this, the second term \(-\frac{1}{2}p^T_{α,⊥} Q(α)p_{α,⊥} + v^T(α)p_{α,⊥} \) is unchanged with respect to the initialization, i.e., one has
\[
-\frac{1}{2}p^T_{α,⊥} Q(α)p_{α,⊥} + v^T(α)p_{α,⊥} = -\frac{1}{2}(p^{(0)}_{α,⊥})^T Q(α)p^{(0)}_{α,⊥} + v^T(α)p^{(0)}_{α,⊥},
\]
(34)
during the maximization process above;

6) In the last part of the analysis, we consider separately the following cases:

a. We first make the simplifying assumption \( v_1 = v_2 = v(α) = 0_n \). In this case, the identity (34) reduces to
\[
-\frac{1}{2}p^T_{α,⊥} Q(α)p_{α,⊥} = -\frac{1}{2}(p^{(0)}_{α,⊥})^T Q(α)p^{(0)}_{α,⊥},
\]
(35)
and \( p^o_{α,⊥} = 0_n \). By considering several random initializations \( p^{(0)} \), one can easily make the term (35) be nearly equal to 0 with high probability. This is made easier by the fact that the discarded principal directions of \( C^{(α)}(α) = Q^2(α) \) are associated with the smallest eigenvalues of \( Q^2(α) \) (hence, also with the smallest eigenvalues of the symmetric and positive definite matrix \( Q(α) \));

b. A similar case as above arises when \( v(α) \neq 0_n \) but \( v(α) \) belongs to the subspace generated by the first \( d \) principal directions of \( C^{(α)}(α) \), because in this case one has \( v^T(α)p_{α,⊥} = 0 \) for any choice of \( p_{α,⊥} \);
c. When cases a) and b) do not hold, it is more difficult to get near the maximum value of the second term (34) by using a multi-start optimization approach. This depends on the fact that on the subspace to which \( p_{\alpha,\perp} \) belongs, the objective function could be almost linear (at least for a small Euclidean norm \( \|p_{\alpha,\perp}\|_2 \)), having only a small quadratic dependence (as that subspace is associated with the smallest eigenvalues of \( Q(\alpha) \)). Hence, in order to make the multi-start optimization approach work fine likewise in cases a) and b) above, a larger number of random initializations would be needed, and sampling of \( p(0) \) should be performed even on a larger domain. Another possible solution – which we have adopted in [8] to deal with a single-objective (non-quadratic and constrained) optimization problem, and in [3] with its multi-objective extension, in both cases with excellent numerical results – consists in using a different construction of \( p_{\alpha,\parallel} \) and \( p_{\alpha,\perp} \). More specifically, one can replace the matrix \( P(\alpha) \) by the orthogonal projection matrix onto the subspace generated by the first \( d \) principal directions and also by the mean gradient \( v(\alpha) \) (or its empirical average).

Although the analysis above has been made for a quite simple multi-objective optimization problem, which can be even solved in closed form, this analysis is expected to be a useful starting point for a future theoretical investigation of the behavior of PCA applied to sampled gradient fields for more complex (both single-objective and multi-objective) optimization problems. It is also worth mentioning that, in the constrained case, a gradient-based optimization algorithm which relies on a PCA approximation of the gradient is more flexible than in the unconstrained one, because it can occasionally move along a subspace different from the one identified by PCA (i.e., when the boundary of the admissible region of the optimization problem is met [8]).

5.2. Multi-objective optimal design of mechanical metamaterial filters. We conclude mentioning that, in our related work [8] about the design of mechanical metamaterial filters according to a single-objective optimization framework\(^7\) (see [19] for a physical-mathematical model similar to the one considered in [8]), we have successfully applied PCA to the sampled gradient field of the objective function, achieving numerical results comparable with those obtained by using the exact gradient, but with a much smaller computational effort (e.g., with a reduction of the dimension by a factor 4). A similar outcome arises when moving to a multi-objective optimization framework, still in the context of mechanical metamaterial filter design. This is the subject of investigation of our ongoing work [3]. So, for the case of the multi-objective optimal design of mechanical metamaterial filters, the application of PCA to the approximation of the sampled gradient field of a suitable associated single-objective function (which represents a proper trade-off between two or more different objectives) can be a valid alternative to the use of surrogate optimization methods (which replace the original objective function with a surrogate function, learned either offline [4] or online [2]), in case a gradient-based optimization algorithm is used to solve the optimization problem. It is also worth mentioning that this particular application of PCA to the multi-objective optimal

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\(^7\)Such optimization problems are typically characterized by a high computational effort needed for an exact evaluation of the gradient of their objective functions, which is motivated by the fact that each such evaluation requires solving the physical-mathematical model associated with the specific choice of the vector of parameters of the model, which is also the vector of optimization variables. The reader is referred to [4] for a further discussion about these computational issues.
design of mechanical metamaterial filters, combined with a multi-start optimization approach, has been the source of inspiration for the theoretical investigation made in the present article.

In the following, we just provide a brief overview of the kind of multi-objective optimization problems arising in the design of mechanical metamaterial filters, in order to show the practical importance of this application. More details about how PCA can be performed on the sampled gradient field of the associated single-objective function in connection with a multi-start optimization algorithm are provided in [8]. The reader is also referred to [19] for the complete description of the underlying physical-mathematical model of [3]. In [19], free and forced wave propagation in beam lattice metamaterials with viscoelastic resonators were investigated. Here, we focus on the Floquet-Bloch spectrum related to free wave propagation. For illustrative purposes, Fig. 2 reports the periodic structure of these metamaterials and of their reference periodic cell.

In this context, recalling the notation used at the beginning of Section 5, the vector $\mathbf{p}$ of optimization variables represents a collection of geometrical/mechanical parameters of the reference periodic cell of a metamaterial, and the functions $J_1(\mathbf{p})$ and $J_2(\mathbf{p})$ can represent, respectively – likewise in the application considered in [3] –, the low-frequency band gap between two specific consecutive dispersion curves in the Floquet-Bloch spectrum of the periodic metamaterial, and the frequency bandwidth of the pass band associated with the three highest-frequency curves of that spectrum. The two objective functions $J_1(\mathbf{p})$ and $J_2(\mathbf{p})$ can be either maximized separately, subject to suitable constraints (possibly included as a penalization term inside each objective function). As an alternative, the trade-off $J_\alpha(\mathbf{p}) = \alpha J_1(\mathbf{p}) + (1 - \alpha) J_2(\mathbf{p})$ can be maximized, subject to the same constraints, for a suitable choice of $\alpha \in [0, 1]$. In the case in which $J_1(\mathbf{p})$, $J_2(\mathbf{p})$ and the constraint functions are assumed to be continuously differentiable, such optimization problems could be numerically solved, e.g., using a gradient-based optimization algorithm, combined with a penalization of the constraints. Differently, in the case in which at least one of them is not continuously differentiable, it is assumed that it can be well-approximated by a continuously differentiable function (e.g., by using a mollifier). In this case, the gradient of the approximating function is actually
considered when a gradient-based optimization algorithm is applied to solve the optimization problems above.

As an example, Figs. 3, 4, and 5 illustrate (by considering two different views for each figure) the resulting optimal Floquet-Bloch spectrum, for each of the three cases. In the figures, $\xi$ denotes the curvilinear abscissa spanning the boundary of a suitable subdomain of the nondimensional first Brillouin zone, whereas $\tilde{s}_n$ denotes the normalized complex eigenfrequency (whose real and imaginary parts are denoted, respectively, as $\mathcal{R}(\tilde{s}_n)$ and $\mathcal{I}(\tilde{s}_n)$).

![Figure 3. Floquet-Bloch spectrum maximizing a low-frequency band gap of a mechanical metamaterial filter: (a) 3-dimensional representation; (b) projection of the spectrum onto a vertical plane.](image)

6. Possible extensions and other applications. The analysis of unconstrained multi-objective maximization with quadratic and concave objective functions, which has been presented in Subsection 5.1, could be extended to more complex multi-objective optimization problems, characterized by the presence of constraints and/or nonquadratic objective functions. To do this, in the latter case, the analysis may be partially reduced to the one of Subsection 5.1, by assuming that PCA is applied in an adaptive way: e.g., based on a subset of gradients sampled in a neighborhood of the current value of the vector of optimization variables, and possibly applying adaptive local quadratic and concave approximations of the objective functions. As another possible development, the theoretical analysis made in the present article could be extended to the application of PCA to the convex combination of more than two data matrices. Another possible extension deals with the case in which PCA is replaced by one of its nonlinear versions, such as kernel PCA [9]. Such an extension seems possible, e.g., via an application of the so-called kernel trick of kernel machines [15].
Figure 4. Floquet-Bloch spectrum maximizing a high-frequency pass band of a mechanical metamaterial filter: (a) 3-dimensional representation; (b) projection of the spectrum onto a vertical plane.

Figure 5. Floquet-Bloch spectrum maximizing a trade-off between a low-frequency band gap and a high-frequency pass band of a mechanical metamaterial filter: (a) 3-dimensional representation; (b) projection of the spectrum onto a vertical plane.

Apart from multi-objective optimization, another interesting possible application of the theoretical analysis made in the present work deals with the case in which PCA is performed on the sampled gradient field of the convex combination of two
images (which is used in image processing, e.g., in order to generate blending effects [5]). In connection to this, it has to be mentioned that applications of PCA to image gradient orientations are reported in [17, 18].

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