

Research Article

Construction of a Class of Sharp Löwner Majorants for a Set of Symmetric Matrices

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The Löwner partial order is taken into consideration in order to define Löwner majorants for a given finite set of symmetric matrices. A special class of Löwner majorants is analyzed based on two specific matrix parametrizations: a two-parametric form and a four-parametric form, which arise in the context of so-called zeroth-order bounds of the effective linear behavior in the field of solid mechanics in engineering. The condensed explicit conditions defining the convex parameter sets of Löwner majorants are derived. Examples are provided, and potential application to semidefinite programming problems is discussed. Open-source MATLAB software is provided to support the theoretical findings and for reproduction of the presented results. The results of the present work offer in combination with the theory of zeroth-order bounds of mechanics a highly efficient approach for the automated material selection for future engineering applications.

1. Introduction

The Löwner partial order introduced by [1] is connected to several matrix partial orders. It implies several matrix inequalities and has been widely studied (see, e.g., [2–6]). This matrix partial order is specifically important for linear and nonlinear optimization problems in semidefinite programming (see, e.g., [7–14]) since it describes an essential part of the constraints in many real-world optimization problems.

In the field of materials science, semidefinite programming problems arise, e.g., in the context of zeroth-order bounds of linear elastic properties of solids. The zeroth-order bounds were introduced by [15] in the context of statistical bounds of linear elastic properties, further analyzed by [16], and corrected by [17, 18]. For instance, an N -phase solid is constituted of N materials with corresponding symmetric positive-definite stiffness matrices, say, $\underline{A}^{(1)}, \dots, \underline{A}^{(N)} \in \mathbb{R}^{n \times n}$ with $n = 6$ for three-dimensional linear elasticity. A zeroth-order bound of the effective linear material behavior of the N -phase solid is a symmetric matrix $\underline{B} \in \mathbb{R}^{n \times n}$ which satisfies

$0 \leq \underline{x}^T (\underline{B} - \underline{A}^{(i)}) \underline{x}, \forall \underline{x} \in \mathbb{R}^n, \forall i \in \{1, \dots, N\}$ for all possible realizations of the solid. In solid mechanics, from realization to realization of a composite material, the orientation of the material constituents may change, i.e., the direction of the eigensystem of each of the stiffnesses $\underline{A}^{(i)}$ can vary from realization to realization. For practical reasons, see, e.g., [17] or [19] for details, the zeroth-order bound is chosen as an isotropic stiffness such that the orientation of the eigensystems of the stiffnesses $\underline{A}^{(i)}$ may not be identical but can at least be fixed. Then, an optimal zeroth-order bound is chosen through the minimization of a, in general, nonlinear function $\varphi(\underline{\beta})$ depending on parameters $\underline{\beta}$ of $\underline{B} = \underline{B}(\underline{\beta})$, cf. [17] for a discussion. This yields the minimization problem

$$\min_{\underline{\beta}} \varphi(\underline{\beta}) \text{ such that } 0 \leq \underline{x}^T (\underline{B}(\underline{\beta}) - \underline{A}^{(i)}) \underline{x}, \quad (1)$$

$$\forall \underline{x} \in \mathbb{R}^n \forall i \in \{1, \dots, N\},$$

which is a classical, in general, nonlinear semidefinite programming problem. Of course, this optimization

problem can be tackled with a high number of general techniques of semidefinite programming. But, since the zeroth-order bounds are chosen as isotropic, the number of free components of $\underline{\underline{B}}(\beta)$ reduces significantly, in linear elasticity to two, and the structure of $\underline{\underline{B}}(\beta)$ is highly specific. An analogous problem can be formulated for linear thermoelasticity, cf. [19], where the number of parameters is four. The low number of parameters in these problems immediately suggests to condense the optimization constraints to a couple of explicit conditions in terms of the parameters β , which are then easily and more efficiently treatable with standard methods. This would significantly reduce the computational time of the optimization problem defining the zeroth-order bounds. This efficiency perspective is particularly of practical importance since, as described in [19], large material databases for solids with multiple constituents could then be scanned, greatly benefiting the material selection in material design problems of engineering applications. This is not only relevant for linear elasticity but also for many associated physical problems, e.g., linear heat or electric conductivity, see, e.g., [20, 21] or [16], such that an investigation of the optimization problem defining the zeroth-order bounds in elasticity would greatly benefit all associated physical problems and corresponding material selection approaches.

The focus of the present work is the proper algebraic analysis and condensation of the optimization constraints to more easily treatable explicit conditions for the two- and four-parametric forms $\underline{\underline{B}}(\beta)$. This parameter constraint condensation has not been conducted in either [15–18] or [19]. For the present investigation, the Löwner partial order is considered, and the concept of Löwner majorants of a single matrix—representing, e.g., a single stiffness matrix—and of a finite matrix set—corresponding to the set of material stiffnesses of a composite material—is introduced. The derived explicit conditions for the parameters β offer compact results which allow to solve nonlinear semidefinite programming problems over the set of resulting Löwner majorants. Most importantly, the evaluation of the constraints is independent of the matrix dimension (modulo a once in a lifetime setup cost that can be performed before the optimization initiation), and it does not require repeated evaluation of subdeterminants of matrices. Additionally, a deterministic construction of the solution is possible for linear cost functions that are of complexity $\mathcal{O}(N)$ for the two-parametric case. Furthermore, geometric interpretations of the stationary condition are provided. The parametrizations are kept as general as possible such that the results of the present work may be of use for other semidefinite programming problems as an efficient generator of simplified solutions or initial guesses.

The manuscript is structured as follows: In Section 2, Löwner majorants of a single symmetric matrix and finite set of symmetric matrices are defined. The two-parametric form is investigated in Section 3, and the explicit conditions defining all corresponding majorants are derived. Examples for the parameter sets of the two-parametric Löwner majorants are given at the end of the section. Then, in Section 4, the four-parametric form is examined building

upon the results of Section 3. Examples for the parameter sets of the Löwner majorants are demonstrated at the end of the section. Furthermore, Section 5 shows an example application of the results in nonlinear semidefinite programming problems and shortly discusses the importance of the examination of the optimization domain and functions to be optimized, since the existence of a minimum is not always assured, even for convex optimization domains and convex functions. Conclusions and potential applications are discussed in Section 6. For full transparency, the authors offer through the GitHub repository [22]

<https://github.com/EMMA-Group/LoewnerMajorant>

open-source MATLAB software containing all programs and data required for the reproduction of all shown examples of the present work.

Notation. Throughout this manuscript, the set of real numbers is denoted by \mathbb{R} . Column vectors over \mathbb{R}^n , $n \in \{2, 3, \dots\}$, are denoted by single-underlined characters, e.g., $\underline{x}, \underline{y}$. Rectangular matrices over $\mathbb{R}^{m \times n}$ are denoted by double-underlined characters, e.g., $\underline{\underline{A}}, \underline{\underline{B}}$. Square matrices over $\mathbb{R}^{n \times n}$ are referred to as matrices of order n . The set of symmetric matrices of order n with finite eigenvalues is denoted by \mathcal{S}_n . The transposition is denoted by the superscript $(\cdot)^T$, e.g., $\underline{a}^T \underline{b}$ equals the scalar product of the vectors, and $\underline{a} \underline{b}^T$ yields the outer product of the vectors. The eigenvalues of a symmetric matrix $\underline{\underline{A}}$ are denoted by $\lambda_i(\underline{\underline{A}}) \in \mathbb{R}$ with $i = 1, \dots, n$. The multiplicity of an eigenvalue λ is denoted as m_λ . The l^2 norm of a vector \underline{a} and the Frobenius norm of a matrix $\underline{\underline{A}}$ are simply noted as $\|\underline{a}\|$ and $\|\underline{\underline{A}}\|$. The identity matrix is noted as $\underline{\underline{I}}$. For a compact notation, the orthogonality of two vectors \underline{p} and \underline{q} or two vector spaces \mathcal{P} and \mathcal{Q} is denoted simply as $\underline{p} \perp \underline{q}$ and $\mathcal{P} \perp \mathcal{Q}$, respectively. The Moore–Penrose inverse of a matrix is denoted by $\underline{\underline{A}}^+$.

2. Löwner Order and Majorants for Symmetric Matrices

In this work, we consider the Löwner partial order of symmetric matrices $\underline{\underline{A}}, \underline{\underline{B}} \in \mathcal{S}_n$ (see, e.g., [6]):

$$\begin{aligned} \underline{\underline{A}} \leq \underline{\underline{B}} &\iff 0 \leq \underline{x}^T (\underline{\underline{B}} - \underline{\underline{A}}) \underline{x}, \quad \forall \underline{x} \in \mathbb{R}^n \\ &\iff \underline{\underline{B}} - \underline{\underline{A}} \in \mathcal{S}_n^+, \end{aligned} \quad (2)$$

where $\mathcal{S}_n^+ \subset \mathcal{S}_n$ denotes the positive semidefinite cone. Any $\underline{\underline{B}} \in \mathcal{S}_n$ is referred to, in this work, as a (Löwner) majorant of a given $\underline{\underline{A}} \in \mathcal{S}_n$ if $\underline{\underline{A}} \leq \underline{\underline{B}}$ holds. Furthermore, any $\underline{\underline{B}} \in \mathcal{S}_n$ is referred to as a sharp (Löwner) majorant of a given $\underline{\underline{A}} \in \mathcal{S}_n$ if $\underline{\underline{A}} \leq \underline{\underline{B}}$ and $\det(\underline{\underline{B}} - \underline{\underline{A}}) = 0$ hold, i.e., if $\underline{\underline{B}} - \underline{\underline{A}} \in \partial \mathcal{S}_n^+$ holds. For given $\underline{\underline{A}} \in \mathcal{S}_n$, the corresponding majorant set $\mathcal{B} \subset \mathbb{R}^{n \times n}$ and sharp majorant set $\partial \mathcal{B}$ are denoted as

$$\begin{aligned} \mathcal{B} &= \{ \underline{\underline{B}} \in \mathcal{S}_n : \underline{\underline{A}} \leq \underline{\underline{B}} \}, \\ \partial \mathcal{B} &= \{ \underline{\underline{B}} \in \mathcal{S}_n : \underline{\underline{A}} \leq \underline{\underline{B}} \wedge \det(\underline{\underline{B}} - \underline{\underline{A}}) = 0 \}. \end{aligned} \quad (3)$$

Of course, \mathcal{B} is nonempty, unbounded, and convex. The trivial majorant $\underline{\underline{T}} \in \partial \mathcal{B}$ of a given $\underline{\underline{A}}$ is defined as

$$\underline{T} = \Lambda_1 \underline{I}, \quad \Lambda_1 = \max_i \lambda_i(\underline{A}). \quad (4)$$

For a finite set $\mathcal{A} = \{\underline{A}^{(1)}, \dots, \underline{A}^{(N)}\}$ of symmetric matrices, we define the analogous majorant set

$$\mathcal{B}^{\mathcal{A}} = \bigcap_{i=1}^N \{\underline{B} \in \mathcal{S}_n: \underline{A}^{(i)} \leq \underline{B}\} = \{\underline{B} \in \mathcal{S}_n: \underline{A} \leq \underline{B} \vee \underline{A} \in \mathcal{A}\}, \quad (5)$$

whose boundary $\partial \mathcal{B}^{\mathcal{A}}$ represents the set of all sharp majorants of \mathcal{A} :

$$\partial \mathcal{B}^{\mathcal{A}} = \{\underline{B} \in \mathcal{S}_n: \underline{A} \leq \underline{B} \vee \underline{A} \in \mathcal{A} \wedge \exists \underline{A} \in \mathcal{A}: \det(\underline{B} - \underline{A}) = 0\}. \quad (6)$$

The trivial element on $\partial \mathcal{B}^{\mathcal{A}}$ is

$$\underline{T}_{\mathcal{A}} = \Lambda_{1,\mathcal{A}} \underline{I}, \quad \Lambda_{1,\mathcal{A}} = \max_{\underline{A} \in \mathcal{A}} \max_i \lambda_i(\underline{A}). \quad (7)$$

3. Two-Parametric Majorant

3.1. Construction of Two-Parametric Majorants for a Single Matrix. For given $\underline{A} \in \mathcal{S}_n$, from the corresponding majorant set \mathcal{B} , we investigate a two-parametric form with given (i.e., fixed) normalized vector $\underline{p}_0 \in \mathbb{R}^n$, $\underline{p}_0 = 1$, defined as a rank-one perturbation of a scaled identity via

$$\underline{B}_2^0 = \beta_1 \underline{I} + \beta_2 \underline{p}_0 \underline{p}_0^T \in \mathcal{S}_n, \quad \underline{\beta} = (\beta_1, \beta_2)^T \in \mathbb{R}^2. \quad (8)$$

In the context of zeroth-order bounds of the effective linear elastic behavior of solid materials, $\underline{p}_0 = (1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3}, 0, 0, 0)$ is given for isotropic zeroth-order bounds if a specific parametrization is chosen, cf., e.g., [16] or [17] for details.

The goal of this section is the derivation of condensed conditions for the parameters $\underline{\beta}$ such that $\underline{B}_2^0 \in \mathcal{B}$ holds. For the sake of a clearer perspective in this section, we consider the spectral factorization of the given $\underline{A} = \underline{U} \underline{\Lambda} \underline{U}^T$ with ordered eigenvalue diagonal matrix $\underline{\Lambda}$ with diagonal entries

$$\Lambda_1 = \Lambda_{11} \geq \Lambda_2 = \Lambda_{22} \geq \dots \geq \Lambda_n = \Lambda_{nn}, \quad (9)$$

and corresponding orthogonal eigenvector matrix \underline{U} , i.e., $\underline{U} \underline{U}^T = \underline{U}^T \underline{U} = \underline{I}$. We denote the set of eigenvectors of \underline{A} as \mathcal{E} and the space of eigenvectors corresponding to a particular eigenvalue as \mathcal{E}_i , i.e.,

$$\begin{aligned} \mathcal{E} &= \{\underline{x} \in \mathbb{R}^n: \underline{\Lambda} \underline{x} = \Lambda \underline{x}, \Lambda \in \{\Lambda_1, \dots\}\}, \\ \mathcal{E}_i &= \{\underline{x} \in \mathbb{R}^n: \underline{\Lambda} \underline{x} = \Lambda_i \underline{x}\}, \quad i = 1, 2, \dots, n. \end{aligned} \quad (10)$$

A change of basis does not alter the Löwner partial order, i.e., $\underline{A} \leq \underline{B}_2^0 \iff \underline{\Lambda} \leq \underline{U}^T \underline{B}_2^0 \underline{U}$. We, therefore, define

$$\underline{B}_2 = \underline{U}^T \underline{B}_2^0 \underline{U} = \beta_1 \underline{I} + \beta_2 \underline{p} \underline{p}^T, \quad \underline{p} = \underline{U}^T \underline{p}_0, \quad (11)$$

and note $\|\underline{p}\| = \|\underline{p}_0\| = 1$. For the remainder of this section, we seek the conditions on the parameters $\underline{\beta} = (\beta_1, \beta_2)$ describing the parameter set

$$\mathcal{B}_2 = \{\underline{\beta} \in \mathbb{R}^2: \underline{\Lambda} \leq \underline{B}_2\}. \quad (12)$$

Due to linear dependency of \underline{B}_2 on $\underline{\beta}$ and the general properties of $\mathcal{B} \subset \mathbb{R}^{n \times n}$, the parameter set $\mathcal{B}_2 \subset \mathbb{R}^2$ is

nonempty, unbounded, and convex. Note that $\underline{\beta} \in \partial \mathcal{B}_2 \iff \underline{B}_2^0(\underline{\beta}) \in \partial \mathcal{B}$ holds.

Due to the length and technical nature of several passages and proofs, the current section is:

- (i) Preparations: introduction of several expressions and relations needed for all following lemmas and remarks
- (ii) Lemma 1: closed form description of \mathcal{B}_2 for $\underline{p} \in \mathcal{E}$
- (iii) Remark 1: remarks for cases on $\partial \mathcal{B}_2$ for Lemma 1
- (iv) Lemma 2: closed form description of \mathcal{B}_2 for $\underline{p} \notin \mathcal{E}$ and β_1 bounded from below by Λ_1 or Λ_2
- (v) Remark 2: remarks for cases on $\partial \mathcal{B}_2$ for Lemma 2
- (vi) Lemma 3: closed form description of \mathcal{B}_2 for $\underline{p} \in \mathcal{E}$ and β_1 bounded from below by a constant between Λ_1 and Λ_2
- (vii) Corollary 1: recapitulation of some topological properties of \mathcal{B}_2 relevant for semidefinite programming problems
- (viii) Remark 3: remarks for cases on $\partial \mathcal{B}_2$ for Lemma 3
- (ix) Remark 4: summarizing remarks and perspective for corresponding semidefinite programming problems

Preparations. Before we derive the conditions describing \mathcal{B}_2 in (12), we introduce some quantities and relations needed throughout this section. The condition $\underline{\Lambda} \leq \underline{B}_2$ is equivalent to the positive semidefiniteness of the difference matrix \underline{C} :

$$\begin{aligned} \underline{C} &= \underline{B}_2 - \underline{\Lambda} = \underline{D} + \beta_2 \underline{p} \underline{p}^T, \\ \underline{D} &= \beta_1 \underline{I} - \underline{\Lambda}, \end{aligned} \quad (13)$$

i.e.,

$$0 \leq \underline{x}^T \underline{C} \underline{x} \quad \forall \underline{x} \in \mathbb{R}^n. \quad (14)$$

We denote the dimension of the kernel of the difference matrix \underline{C} as

$$\kappa = \dim(\ker(\underline{C})). \quad (15)$$

We define the mutually orthogonal vector spaces

$$\begin{aligned} \mathcal{P} &= \text{span}\{\underline{p}\}, \\ \mathcal{Q} &= \{\underline{x} \in \mathbb{R}^n: \underline{x}^T \underline{p} = 0\}, \end{aligned} \quad (16)$$

and introduce a matrix $\underline{Q} \in \mathbb{R}^{n \times (n-1)}$ such that the concatenated matrix $(\underline{p}, \underline{Q}) \in \mathbb{R}^{n \times n}$ is orthogonal, i.e., the columns of \underline{Q} form an orthonormal basis of \mathcal{Q} . We define

$$\begin{aligned} \mu_{\mathcal{P}} &= \underline{p}^T \underline{\Lambda} \underline{p}, \\ \mu_{\mathcal{Q}} &= \max_{\substack{\underline{x} \in \mathcal{Q} \\ \|\underline{x}\|=1}} \underline{x}^T \underline{\Lambda} \underline{x} = \max_{1 \leq i \leq n-1} \lambda_i(\underline{Q}^T \underline{\Lambda} \underline{Q}), \\ c_{\mathcal{Q}} &= \underline{p}^T (\mu_{\mathcal{Q}} \underline{I} - \underline{\Lambda})^+ \underline{p}, \end{aligned} \quad (17)$$

where $\mu_{\mathcal{Q}}$ corresponds to the largest eigenvalue of the reduced matrix $\underline{Q}^T \underline{\Lambda} \underline{Q} \in \mathcal{S}_{n-1}$. Inserting vectors from \mathcal{P} and \mathcal{Q} into (14), respectively, yields the two elementary necessary conditions:

$$\beta_1 + \beta_2 \geq \mu_{\mathcal{P}}, \quad (18)$$

$$\beta_1 \geq \mu_{\mathcal{Q}}. \quad (19)$$

Note that $\mu_{\mathcal{Q}}$ is bounded by Λ_1 due to

$$\Lambda_1 = \max_{\|\underline{x}\|=1} \underline{x}^T \underline{\underline{\Lambda}} \underline{x} \geq \max_{\underline{x} \in \mathcal{Q} \wedge \|\underline{x}\|=1} \underline{x}^T \underline{\underline{\Lambda}} \underline{x} = \mu_{\mathcal{Q}}. \quad (20)$$

Furthermore, the relation

$$\mu_{\mathcal{Q}} \geq \Lambda_2, \quad (21)$$

is obtained based on the following arguments:

- (1) If $\underline{p}^T \underline{e}_1 = 0$, then $\underline{e}_1 \in \mathcal{Q}$ and $\mu_{\mathcal{Q}} = \Lambda_1 \geq \Lambda_2$ holds.
- (2) If $\underline{p}^T \underline{e}_1 \neq 0$, then using $\alpha = (\underline{p}^T \underline{e}_2) / (\underline{p}^T \underline{e}_1)$, one can define $\underline{q} = \underline{e}_2 - \alpha \underline{e}_1 \in \mathcal{Q}$ with $\underline{q}^T \underline{q} = 1 + \alpha^2$. Substituting $\underline{e}_2 = \alpha \underline{e}_1 + \underline{q}$ implies

$$\begin{aligned} \Lambda_2 &= \underline{e}_2^T \underline{\underline{\Lambda}} \underline{e}_2 \\ &= (\alpha \underline{e}_1 + \underline{q})^T (\alpha \Lambda_1 \underline{e}_1 + \underline{\underline{\Lambda}} \underline{q}) \\ &= -\alpha^2 \Lambda_1 + (1 + \alpha^2) \frac{\underline{q}^T \underline{\underline{\Lambda}} \underline{q}}{\underline{q}^T \underline{q}} \end{aligned} \quad (22)$$

$$\stackrel{(17)}{\leq} \mu_{\mathcal{Q}} - \alpha^2 (\Lambda_1 - \mu_{\mathcal{Q}})$$

$$\stackrel{(20)}{\leq} \mu_{\mathcal{Q}}.$$

Therefore,

$$\Lambda_2 \leq \mu_{\mathcal{Q}} \leq \Lambda_1, \quad (23)$$

generally holds. Denote the algebraic multiplicity of the maximum eigenvalue Λ_1 by m_{Λ_1} . It is noted that

$$\mu_{\mathcal{Q}} = \Lambda_1 \iff \mathcal{P} \perp \mathcal{E}_1 \vee m_{\Lambda_1} \geq 2, \quad (24)$$

and based on (22),

$$\mu_{\mathcal{Q}} = \Lambda_2 < \Lambda_1 \implies m_{\Lambda_1} = 1 \wedge \mathcal{P} \perp \mathcal{E}_1 \wedge \mathcal{P} \perp \mathcal{E}_2, \quad (25)$$

holds. Based on these preparations, we now proceed to the description of the parameter set \mathcal{B}_2 through three lemmas.

Lemma 1. *If $\underline{p} \in \mathcal{E}$ holds, then the parameter set \mathcal{B}_2 is described by*

$$\mathcal{B}_2 = \{\underline{\beta} \in \mathbb{R}^2: \beta_1 \geq \mu_{\mathcal{Q}} \wedge \beta_2 \geq \mu_{\mathcal{P}} - \beta_1\}. \quad (26)$$

Proof. If $\underline{p} \in \mathcal{E}$, corresponding to Λ_i for some $i \in \{1, \dots, n\}$, then (18) and (19) simplify to

$$\beta_1 + \beta_2 \geq \mu_{\mathcal{P}} = \Lambda_i, \quad \beta_1 \geq \mu_{\mathcal{Q}} = \max_{j \neq i} \Lambda_j. \quad (27)$$

For this case, (27) is equivalent to $\underline{\underline{\Lambda}} \leq \underline{\underline{B}}_2$ such that \mathcal{B}_2 defined in (12) simplifies to (26). \square

Remark 1. For Lemma 1, all $\underline{\beta} \in \partial \mathcal{B}_2$ (i.e., at least one of the inequalities in (26) turns into an equality) are sharp majorants and induce a singular $\underline{\underline{C}} = \underline{\underline{B}}_2 - \underline{\underline{\Lambda}}$ with nonempty kernel $\ker(\underline{\underline{C}})$ of dimension κ , cf. (15). The special cases for $\underline{\beta} \in \partial \mathcal{B}_2$

$$\begin{aligned} \underline{p} \in \mathcal{E} \wedge m_{\mu_{\mathcal{Q}}} = 1 \wedge \beta_1 = \mu_{\mathcal{Q}} \wedge \beta_2 > \mu_{\mathcal{P}} - \mu_{\mathcal{Q}} \\ \implies \kappa = 1 \wedge \ker(\underline{\underline{C}}) \perp \mathcal{P}, \end{aligned} \quad (28)$$

$$\underline{p} \in \mathcal{E} \wedge \beta_1 > \mu_{\mathcal{Q}} \wedge \beta_2 = \mu_{\mathcal{P}} - \beta_1 \implies \kappa = 1 \wedge \ker(\underline{\underline{C}}) \perp \mathcal{P}, \quad (29)$$

deliver a one-dimensional kernel of $\underline{\underline{C}}$. It is noted that only (29) ensures $\kappa = 1$, independent of the multiplicity $m_{\mu_{\mathcal{Q}}}$ of $\mu_{\mathcal{Q}}$, and, more importantly, that $\ker(\underline{\underline{C}}) \perp \mathcal{P}$ holds. This property is of interest for Section 4.

Lemma 2. *If $\underline{p} \notin \mathcal{E}$ and $\mu_{\mathcal{Q}} \in \{\Lambda_1, \Lambda_2\}$ hold, then the parameter set \mathcal{B}_2 is described:*

- (1) For $\mu_{\mathcal{Q}} = \Lambda_1$ and eigenspace \mathcal{E}_1 corresponding to Λ_1 as

$$\begin{aligned} \mathcal{B}_2 &= \{\underline{\beta} \in \mathbb{R}^2: \mu_{\mathcal{Q}} \leq \beta_1 \wedge \beta_2^{\min} \leq \beta_2\}, \\ \beta_2^{\min} &= \begin{cases} -(\underline{p}^T \underline{\underline{D}}^{-1} \underline{p})^{-1}, & \beta_1 \neq \Lambda_1, \\ -(c_{\mathcal{Q}})^{-1}, & \beta_1 = \Lambda_1 \wedge \mathcal{P} \perp \mathcal{E}_1, \\ 0, & \beta_1 = \Lambda_1 \wedge \mathcal{P} \not\perp \mathcal{E}_1. \end{cases} \end{aligned} \quad (30)$$

- (2) For $\mu_{\mathcal{Q}} = \Lambda_2 < \Lambda_1$ and $c_{\mathcal{Q}} \neq 0$, cf. (17), as

$$\begin{aligned} \mathcal{B}_2 &= \{\underline{\beta} \in \mathbb{R}^2: \mu_{\mathcal{Q}} \leq \beta_1 \wedge \beta_2^{\min} \leq \beta_2\}, \\ \beta_2^{\min} &= \begin{cases} -(\underline{p}^T \underline{\underline{D}}^{-1} \underline{p})^{-1}, & \beta_1 \neq \Lambda_1 \wedge \beta_1 \neq \Lambda_2, \\ 0, & \beta_1 = \Lambda_1, \\ -(c_{\mathcal{Q}})^{-1}, & \beta_1 = \Lambda_2. \end{cases} \end{aligned} \quad (31)$$

- (3) For $\mu_{\mathcal{Q}} = \Lambda_2 < \Lambda_1$ and $c_{\mathcal{Q}} = 0$, cf. (17), as

$$\begin{aligned} \mathcal{B}_2 &= \{\underline{\beta} \in \mathbb{R}^2: \mu_{\mathcal{Q}} < \beta_1 \wedge \beta_2^{\min} \leq \beta_2\}, \\ \beta_2^{\min} &= \begin{cases} -(\underline{p}^T \underline{\underline{D}}^{-1} \underline{p})^{-1}, & \beta_1 \neq \Lambda_1, \\ 0, & \beta_1 = \Lambda_1. \end{cases} \end{aligned} \quad (32)$$

Proof. We investigate the interval $[\mu_{\mathcal{Q}}, \infty)$ for β_1 in \mathcal{B}_2 with $\mu_{\mathcal{Q}} \in \{\Lambda_1, \Lambda_2\}$ based on the following cases:

- (1) $\beta_1 \in (\Lambda_1, \infty)$: In this case, sharp majorants require a singular difference matrix $\underline{\underline{C}} = \underline{\underline{B}}_2 - \underline{\underline{\Lambda}} = \underline{\underline{D}} + \beta_2 \underline{p} \underline{p}^T$. Due to the restriction $\Lambda_1 < \beta_1$ of this case, the diagonal matrix $\underline{\underline{D}} = \beta_1 \underline{I} - \underline{\underline{\Lambda}}$ is positive definite such that, based on the determinant lemma, cf., e.g., [23] or [24], we consider

$$\begin{aligned} 0 &= \det(\underline{\underline{C}}) \\ &= \det(\underline{\underline{D}} + \beta_2 \underline{p} \underline{p}^T) \\ &= \det(\underline{\underline{D}}) (1 + \beta_2 \underline{p}^T \underline{\underline{D}}^{-1} \underline{p}), \end{aligned} \quad (33)$$

which is a single-valued constraint in terms of β_2 with $\underline{p}^T \underline{\underline{D}}^{-1} \underline{p} > 0$. This is fulfilled iff

$$\beta_2 = \frac{1}{\underline{p}^T \underline{D}^{-1} \underline{p}}, \quad (34)$$

meaning that (34) describes for every $\beta_1 \in (\Lambda_1, \infty)$ the corresponding β_2 yielding a sharp majorant, i.e., (34) specifies a portion of $\partial \mathcal{B}_2$. Due to the convexity of \mathcal{B}_2 , $\beta_2 \geq -(\underline{p}^T \underline{D}^{-1} \underline{p})^{-1}$ delivers trivially nonsharp majorants for $\beta_1 \in (\Lambda_1, \infty)$.

- (2) $\beta_1 = \Lambda_1$: the matrix $\underline{D} = \Lambda_1 \underline{I} - \underline{\Lambda}$ is singular and positive semidefinite. We consider the matrices

$$\underline{E}_1 = (\underline{e}_1 \dots \underline{e}_{m_{\Lambda_1}}), \quad \underline{E}_1^\perp = (\underline{e}_{m_{\Lambda_1}+1} \dots \underline{e}_n), \quad (35)$$

which contain in the respective columns a basis of \mathcal{E}_1 for Λ_1 and of the corresponding orthogonal space \mathcal{E}_1^\perp . We examine the following cases:

- (a) If $\mathcal{P} \perp \mathcal{E}_1$ holds, then \underline{C} is already singular, independently of β_2 , since

$$\begin{aligned} \underline{e}_1^T \underline{C} \underline{e}_1 &= \underline{e}_1^T (\Lambda_1 \underline{I} - \underline{\Lambda} + \beta_2 \underline{p} \underline{p}^T) \underline{e}_1 \\ &= \underline{e}_1^T (\Lambda_1 \underline{e}_1 - \underline{\Lambda} \underline{e}_1) = 0, \end{aligned} \quad (36)$$

holds, meaning that $\ker(\underline{C})$ is at least one-dimensional. Based on (35) and $\underline{x} = \underline{E}_1^\perp \underline{\xi}$, $\underline{\xi} \in \mathbb{R}^{n-m_{\Lambda_1}}$, (14) can be further reduced to

$$\begin{aligned} 0 &\leq \underline{\xi}^T \underline{\tilde{C}} \underline{\xi}, \quad \forall \underline{\xi} \in \mathbb{R}^{n-m_{\Lambda_1}}, \\ \underline{\tilde{C}} &= \underline{\tilde{D}} + \beta_2 \underline{\tilde{p}} \underline{\tilde{p}}^T, \\ \underline{\tilde{D}} &= (\underline{E}_1^\perp)^T \underline{D} \underline{E}_1^\perp, \\ \underline{\tilde{p}} &= (\underline{E}_1^\perp)^T \underline{p}. \end{aligned} \quad (37)$$

The matrix $\underline{\tilde{D}}$ is positive definite, and since \underline{p} is not an eigenvector of $\underline{\Lambda}$, $\underline{\tilde{p}} \neq \underline{0}$ holds. For $\underline{\tilde{C}}$ to be singular, its determinant has to vanish. Analogous application of the matrix determinant lemma as in (33) yields that $\underline{\tilde{C}}$ is singular iff

$$\beta_2 = -\frac{1}{\underline{\tilde{p}}^T \underline{\tilde{D}}^{-1} \underline{\tilde{p}}} = -\frac{1}{\underline{p}^T \underline{D}^+ \underline{p}}, \quad (38)$$

where \underline{D}^+ denotes the Moore–Penrose inverse of \underline{D} . The choice (38) induces a second vanishing eigenvalue in \underline{C} such that its kernel is then at least two-dimensional.

- (b) If $\mathcal{P} \not\perp \mathcal{E}_1$ holds, then using (35) and $\underline{x} = \underline{E}_1 \underline{\xi}$, $\underline{\xi} \in \mathbb{R}^{m_{\Lambda_1}}$ in (14) yields the necessary condition

$$\beta_2 \geq 0. \quad (39)$$

This condition is also sufficient for $\underline{\Lambda} \leq \underline{B}_2$. For $\beta_2 = 0$, one retrieves for the current scenario the trivial majorant $\underline{\beta} = (\Lambda_1, 0) \in \partial \mathcal{B}_2$, cf. (4).

If $\mu_{\mathcal{Q}} = \Lambda_1$ holds, cf. (24), then cases 1 and 2 of this proof describe β_2^{\min} , at what $c_{\mathcal{Q}} \neq 0$, cf. (17), is identified in (38), yielding (30)—cf. Lemma 2.1 as depicted in Figure 1 in the

ramification for $\underline{p} \notin \mathcal{E}$ and $\mu_{\mathcal{Q}} = \Lambda_1$. If $\Lambda_2 < \Lambda_1$ and $\mu_{\mathcal{Q}} = \Lambda_2$ hold, cf. (25), then case 1 of this proof still applies, but the following cases relevant for Lemma 2.2 and Lemma 2.3, depicted in Figure 1, also need to be considered:

- (2') $\beta_1 = \Lambda_1$: Due to $\mathcal{P} \not\perp \mathcal{E}_1$, (39) must hold for this case.

- (3') $\beta_1 \in (\Lambda_2, \Lambda_1)$: For the present case, $\underline{D} = \beta_1 \underline{I} - \underline{\Lambda}$ is indefinite and regular such that the determinant lemma can be applied analogously as in (33), but (34) is not immediately clear since the term $\underline{p}^T \underline{D}^{-1} \underline{p}$ may vanish for such indefinite \underline{D} . More precisely, the term $\underline{p}^T \underline{D}^{-1} \underline{p}$ may vanish, iff $\underline{D}^{-1} \underline{p} \in \mathcal{Q}$ holds. We search now for a vector $\underline{q} = \underline{Q} \underline{\xi} \in \mathcal{Q}$ such that $\underline{p} = \underline{D} \underline{q}$ holds, with the necessary condition

$$\begin{aligned} \underline{0} &= \underline{Q}^T \underline{D} \underline{q} \\ &= \underline{Q}^T (\beta_1 \underline{I} - \underline{\Lambda}) \underline{Q} \underline{\xi} \\ &= \beta_1 \underline{\xi} - \underline{Q}^T \underline{\Lambda} \underline{Q} \underline{\xi}. \end{aligned} \quad (40)$$

This means that $\underline{\xi}$ would be required to correspond to the eigenvector of the reduced matrix $\underline{Q}^T \underline{\Lambda} \underline{Q}$ for eigenvalue β_1 . But, we consider β_1 larger than the maximum eigenvalue $\mu_{\mathcal{Q}} = \Lambda_2$ of $\underline{Q}^T \underline{\Lambda} \underline{Q}$ such that no such $\underline{\xi}$ exists, and therefore, the term $\underline{p}^T \underline{D}^{-1} \underline{p}$ cannot vanish. Solving (33) for β_2 yields again (34).

- (4') $\beta_1 = \Lambda_2$: Due to $\mathcal{P} \perp \mathcal{E}_2$, analogous reasoning as in 2(a) is applied to this case with corresponding \underline{E}_2 and \underline{E}_2^\perp up to the corresponding equation

$$\begin{aligned} 0 &\leq \underline{\xi}^T \underline{\tilde{C}} \underline{\xi}, \quad \forall \underline{\xi} \in \mathbb{R}^{n-m_{\Lambda_2}}, \\ \underline{\tilde{C}} &= \underline{\tilde{D}} + \beta_2 \underline{\tilde{p}} \underline{\tilde{p}}^T, \\ \underline{\tilde{D}} &= (\underline{E}_2^\perp)^T \underline{D} \underline{E}_2^\perp, \\ \underline{\tilde{p}} &= (\underline{E}_2^\perp)^T \underline{p}. \end{aligned} \quad (41)$$

The difference to 2(a) here is that $\underline{\tilde{D}}$ is not positive definite but regular and indefinite. For $\underline{\tilde{C}}$ to be singular, its determinant must vanish. Application of the matrix determinant lemma as in (33) yields

$$0 = \det(\underline{\tilde{C}}) = \det(\underline{\tilde{D}}) \left(1 + \beta_2 \underline{\tilde{p}}^T \underline{\tilde{D}}^{-1} \underline{\tilde{p}} \right). \quad (42)$$

Here, the term $\underline{\tilde{p}}^T \underline{\tilde{D}}^{-1} \underline{\tilde{p}} = \underline{p}^T \underline{D}^+ \underline{p}$ equals the quantity $c_{\mathcal{Q}}$ for $\mu_{\mathcal{Q}} = \Lambda_2$, see (17). The quantity $c_{\mathcal{Q}}$ may or may not vanish, depending solely on $\underline{\Lambda}$ and \underline{p} . This means that if $c_{\mathcal{Q}} \neq 0$, then (42) can be solved for β_2 as in (38), yielding $\beta_1 \in [\mu_{\mathcal{Q}}, \infty)$ and (31)—cf. Lemma 2.2 as depicted in Figure 1. But, if $c_{\mathcal{Q}} = 0$ holds, then there exists no β_2 for $\beta_1 = \Lambda_2$ such that $(\beta_1, \beta_2) \in \mathcal{B}_2$ holds since $\det(\underline{\tilde{C}})$ cannot vanish. Therefore, $c_{\mathcal{Q}} = 0$ yields (32) and, more importantly, excludes $\mu_{\mathcal{Q}} = \Lambda_2$ from the range of β_1 for the current scenario, i.e., $\beta_1 \in (\mu_{\mathcal{Q}}, \infty)$, cf. Lemma 2.3 illustrated in Figure 1. \square

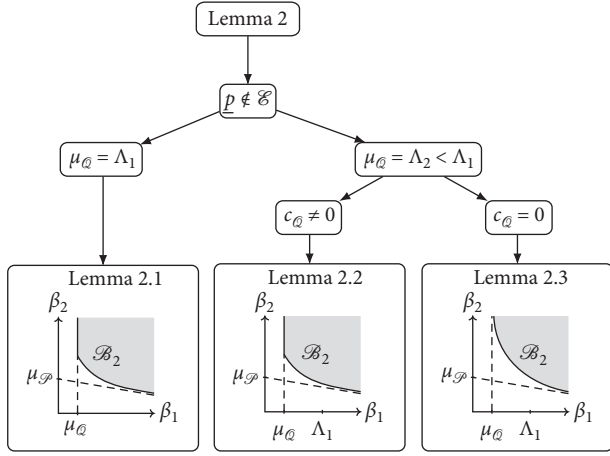


FIGURE 1: Illustration of Lemma 2.

Remark 2. It is noted that, for Lemma 2, $\kappa = 1$, cf. (15), holds in a number of scenarios. In order to visualize the following argument, the position of the upcoming cases in the set \mathcal{B}_2 is depicted in Figure 2.

In cases 1 and 3' of the proof of Lemma 2, the rank-one perturbation $\beta_2 \underline{p} \underline{p}^T$ can only induce a one-dimensional kernel on the difference matrix $\underline{C} = \underline{D} + \beta_2 \underline{p} \underline{p}^T$ with regular \underline{D} for β_2 fulfilling (34). This corresponds to the majority of points described through β_2^{\min} in Lemma 2, only excluding the special case $\beta_1 = \Lambda_1$. The corresponding kernel vector \underline{n} with $\ker(\underline{C}) = \text{span}\{\underline{n}\}$ is obtained as

$$\underline{n} = \underline{D}^{-1} \underline{p} \implies \underline{C} \underline{n} = \underline{D} \underline{n} + (-1) \frac{1}{\underline{p}^T \underline{n}} \underline{p} \underline{p}^T \underline{n} = \underline{o}, \quad (43)$$

such that

$$\underline{p} \notin \mathcal{E} \wedge \mu_Q < \beta_1 \wedge \beta_1 \neq \Lambda_1 \wedge (34) \implies \kappa = 1 \wedge \ker(\underline{C}) \perp \mathcal{P}, \quad (44)$$

holds since $0 \neq \underline{p}^T \underline{n} = \underline{p}^T \underline{D}^{-1} \underline{p}$ holds. The corresponding points $\underline{\beta} \in \partial \mathcal{B}_2$ based on β_2^{\min} inducing (44) are indicated in Figure 2 at the lower border of \mathcal{B}_2 with $\kappa = 1$, and more importantly, due to the consequences of Section 4, $\ker(\underline{C}) \perp \mathcal{P}$.

For $\mu_Q = \Lambda_1$, i.e., Lemma 2.1 is considered, the point at $\beta_1 = \mu_Q = \Lambda_1$ is to be examined. Hereby, cases 2(a) and 2(b) of the proof of Lemma 2 need some attention. In case 2(a), i.e., $\mathcal{P} \perp \mathcal{E}_1$, \underline{C} is already singular ($\underline{C} \underline{e}_1 = \underline{o}$, i.e., $\underline{e}_1 \in \ker(\underline{C})$) and for β_2 fulfilling (38), the rank-one perturbation $\beta_2 \underline{p} \underline{p}^T$ induces a further vanishing eigenvalue of \underline{C} such that $\ker(\underline{C})$ is at least two-dimensional. This special case corresponds to the black point in Figure 2. For β_2 above the critical value given in (38), $\ker(\underline{C})$ is then at least one-dimensional such that $\kappa = 1$ is only possible at $\beta_1 = \mu_Q = \Lambda_1$ under the current assumptions only for $m_{\Lambda_1} = 1$, i.e.,

$$\underline{p} \notin \mathcal{E} \wedge m_{\Lambda_1} = 1 \wedge \mathcal{P} \perp \mathcal{E}_1 \wedge \beta_1 = \Lambda_1 \wedge \beta_2 > -(c_Q)^{-1} \implies \kappa = 1 \wedge \ker(\underline{C}) \perp \mathcal{P}. \quad (45)$$

In case 2(b), i.e., $\mathcal{P} \not\perp \mathcal{E}_1$, \underline{p} is not perpendicular to the complete eigenspace of Λ_1 , but for $m_{\Lambda_1} \geq 2$, there always exists at least one eigenvector to Λ_1 which is perpendicular to

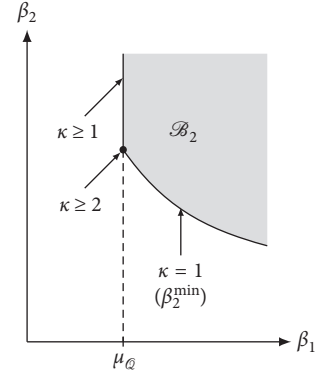


FIGURE 2: Dimension of kernel $\kappa = \dim(\ker(\underline{C}))$ of difference matrix \underline{C} on $\partial \mathcal{B}_2$ for Lemma 2.1 and Lemma 2.2 with $\mu_Q \in \{\Lambda_1, \Lambda_2\}$ and $c_Q \neq 0$; in case of $c_Q = 0$, corresponding to Lemma 2.3, $\partial \mathcal{B}_2$ is described by the curve $\beta_2^{\min}(\beta_1)$ ($\kappa = 1$), which then diverges to $+\infty$ at $\beta_1 = \mu_Q$.

\underline{p} . Therefore, $\kappa = 1$ is only possible at $\beta_1 = \Lambda_1$ under the current assumptions for $m_{\Lambda_1} = 2$, i.e.,

$$\underline{p} \notin \mathcal{E} \wedge m_{\Lambda_1} = 2 \wedge \mathcal{P} \perp \mathcal{E}_1 \wedge \beta_1 = \Lambda_1 \wedge \beta_2 > 0 \implies \kappa = 1 \wedge \ker(\underline{C}) \perp \mathcal{P}. \quad (46)$$

These arguments imply that, for Lemma 2.1, based on (44)–(46), $\kappa = 1$ and $\ker(\underline{C}) \perp \mathcal{P}$ are assured only for points $\underline{\beta} \in \partial \mathcal{B}_2$ corresponding to $\mu_Q = \Lambda_1 < \beta_1$ and $\beta_2 = \beta_2^{\min}(\beta_1)$.

For $\mu_Q = \Lambda_2 < \Lambda_1$, cf. (25), we need to examine the points at $\beta_1 = \Lambda_1$ and $\beta_1 = \Lambda_2 = \mu_Q$ for Lemma 2.2 and Lemma 2.3. For case 2', addressing $\beta = \Lambda_1$,

$$\underline{p} \notin \mathcal{E} \wedge m_{\Lambda_1} = 1 \wedge \mathcal{P} \perp \mathcal{E}_1 \wedge \beta_1 = \Lambda_1 \wedge \beta_2 = 0 \implies \kappa = 1 \wedge \ker(\underline{C}) \perp \mathcal{P}, \quad (47)$$

follows such that, for $\mu_Q < \beta_1$, the lower boundary of \mathcal{B}_2 depicted in Figure 2 yields $\kappa = 1$ and $\ker(\underline{C}) \perp \mathcal{P}$. Analogous reasoning as for (45) yields for case 4', addressing $\beta_1 = \Lambda_2 = \mu_Q$,

$$\underline{p} \notin \mathcal{E} \wedge \mu_Q = \Lambda_2 < \Lambda_1 \wedge c_Q \neq 0 \wedge m_{\Lambda_2} = 1 \wedge \beta_1 = \Lambda_2 \wedge \beta_2 > -(c_Q)^{-1} \implies \kappa = 1 \wedge \ker(\underline{C}) \perp \mathcal{P}. \quad (48)$$

It can be concluded for Lemma 2 that only for $\mu_Q < \beta_1$ and $\underline{\beta} \in \partial \mathcal{B}_2$, the kernel of \underline{C} stays one-dimensional (indicated in Figure 2 by the border with $\kappa = 1$) and, more importantly, that $\ker(\underline{C}) \perp \mathcal{P}$ holds. This property is of interest for Section 4.

Lemma 3. If $\underline{p} \notin \mathcal{E}$ and $\Lambda_2 < \mu_Q < \Lambda_1$ hold, then the parameter set \mathcal{B}_2 is described by

$$\mathcal{B}_2 = \{\underline{\beta} \in \mathbb{R}^2: \mu_Q < \beta_1 \wedge \beta_2^{\min} \leq \beta_2\}, \quad \beta_2^{\min} = \begin{cases} -(p^T \underline{D}^{-1} p)^{-1}, & \beta_1 \neq \Lambda_1, \\ 0, & \beta_1 = \Lambda_1. \end{cases} \quad (49)$$

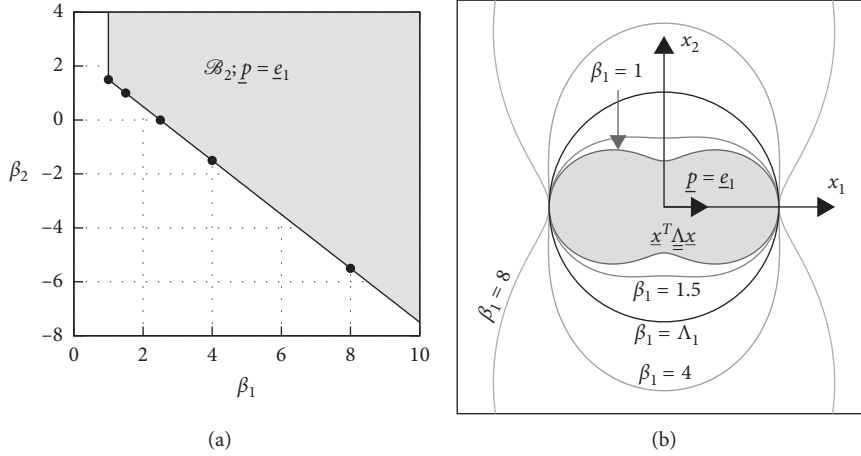


FIGURE 3: (a) Parameter region \mathcal{B}_2 for \underline{A} and \underline{p}_1 ; (b) isolines of the quadratic forms $\underline{x}^T \underline{A} \underline{x}$ and $\underline{x}^T \underline{B}_2 \underline{x}$ in the (1,2)-plane for all normalized \underline{x} for the marked black points of (a).

Consideration of \underline{p}_2 yields an instance of Lemma 2 (\underline{p} is not an eigenvector of \underline{A} , $m_{\Lambda_1} = 1$, and $\underline{p}^T \underline{e}_1 = 0$, i.e., $\mu_{\mathcal{Q}} = \Lambda_1$). The corresponding results are depicted in Figure 4. It should be noted that, for $\beta_1 = \mu_{\mathcal{Q}} = \Lambda_1$, the pseudoinverse of \underline{D} is required and $c_{\mathcal{Q}}$ is evaluated, while for $\beta_1 > \mu_{\mathcal{Q}}$, the inverse of \underline{D} is computed. In Figure 4(b), the region around $\beta_1 = \Lambda_1$ is shown more clearly. The contour plots in Figures 4(c) and 4(d) indicate the difference between the majorant and the original matrix, with the second plot showing that all contours of Figure 4(c) in fact have a contact point with the original hypersurface (drawn as dashed line) outside of the (1,2)-plane, cf. Figure 4(d).

Lastly, \underline{p}_3 is an instance of Lemma 3 (\underline{p} is not an eigenvector of \underline{A} and $\Lambda_2 < \mu_{\mathcal{Q}} < \Lambda_1$), with corresponding results depicted in Figure 5. Most notably, the value $\beta_1 = \mu_{\mathcal{Q}}$ marks the asymptote of the boundary of \mathcal{B}_2 since for $\beta_1 = \mu_{\mathcal{Q}}$, no β_2 exists yielding a point on $\partial \mathcal{B}_2$, cf. case 4 of the proof of Lemma 3.

3.4. Example: Majorization of a Set of Matrices. Consider the finite set of symmetric matrices

$$\mathcal{A} = \{ \underline{A}^{(1)}, \underline{A}^{(2)} \},$$

$$\underline{A}^{(1)} = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -3 \end{pmatrix}, \tag{58}$$

$$\underline{A}^{(2)} = \frac{1}{9} \begin{pmatrix} -4 & 14 & -16 \\ 14 & 5 & 2 \\ -16 & 2 & -10 \end{pmatrix},$$

and the vector

$$\underline{p}_0 = (1, 0, 0)^T. \tag{59}$$

The border of the corresponding set $\mathcal{B}_2^{(1)}$ (an instance of Lemma 1) is depicted in Figure 6 by the straight lines. The border of the corresponding $\mathcal{B}_2^{(2)}$ (an instance of Lemma 3) is depicted by the curved black line in Figure 6. The majorant set $\mathcal{B}_2^{\mathcal{A}}$ defined in (56) is depicted in Figure 6 by the gray region. The depicted region can be reproduced with the file

demo2.m

using the provided MATLAB software, cf. [22].

Next, a set of $N = 10$ random symmetric matrices of dimension $n = 100$ is generated. The intersection of the critical domains is shown in Figure 7 as well as the curves denoting the boundaries of the critical domain for each matrix $\underline{A}^{(i)}$ of the set. Close inspection of the graph shows that there are multiple intersections of these lines which generate the boundary of the overall critical domain $\mathcal{B}_2^{\mathcal{A}}$.

4. Four-Parametric Majorant

4.1. Construction of Four-Parametric Majorant for a Single Matrix. In addition to the two-parametric majorant of Section 3, a four-parametric majorant is examined in this section. A given $\underline{A}_4 \in \mathcal{S}_{n+1}$ is considered and partitioned as follows:

$$\underline{A}_4 = \begin{pmatrix} \underline{A} & \underline{a} \\ \underline{a}^T & a_0 \end{pmatrix} \in \mathcal{S}_{n+1}, \quad \underline{A} \in \mathcal{S}_n, \quad \underline{a} \in \mathbb{R}^n, \quad a_0 \in \mathbb{R}. \tag{60}$$

From all majorants of \underline{A}_4 , we are interested in this section in the parametrization

$$\underline{B}_4^0 = \begin{pmatrix} \beta_1 \underline{I} + \beta_2 \underline{p}_0 \underline{p}_0^T & \beta_4 \underline{p}_0 \\ \beta_4 \underline{p}_0^T & \beta_3 \end{pmatrix} \in \mathcal{S}_{n+1}, \tag{61}$$

with given normalized \underline{p}_0 . This four-parametric form arises in linear thermo-elasticity and corresponding isotropic zeroth-order bounds, cf. [19]. The upper left block of \underline{B}_4^0 corresponds to

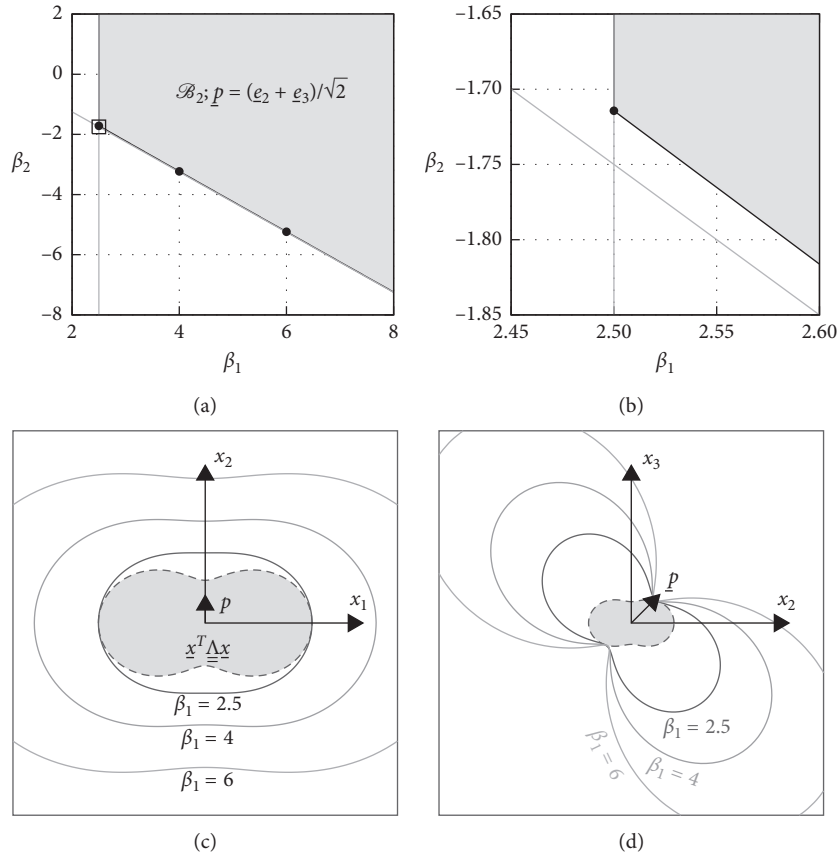


FIGURE 4: (a) Parameter region \mathcal{B}_2 for \underline{A} and \underline{p}_2 ; (b) zoomed region around $\beta_1 = \Lambda_1 = 5/2$ marked with the black rectangle in (a); (c) isolines of the quadratic forms $\underline{x}^T \underline{A} \underline{x}$ and $\underline{x}^T \underline{B}_2 \underline{x}$ in the $(1,2)$ -plane for all normalized \underline{x} for the marked black points of (a); (d) evaluation of the quadratic forms in the $(2,3)$ -plane.

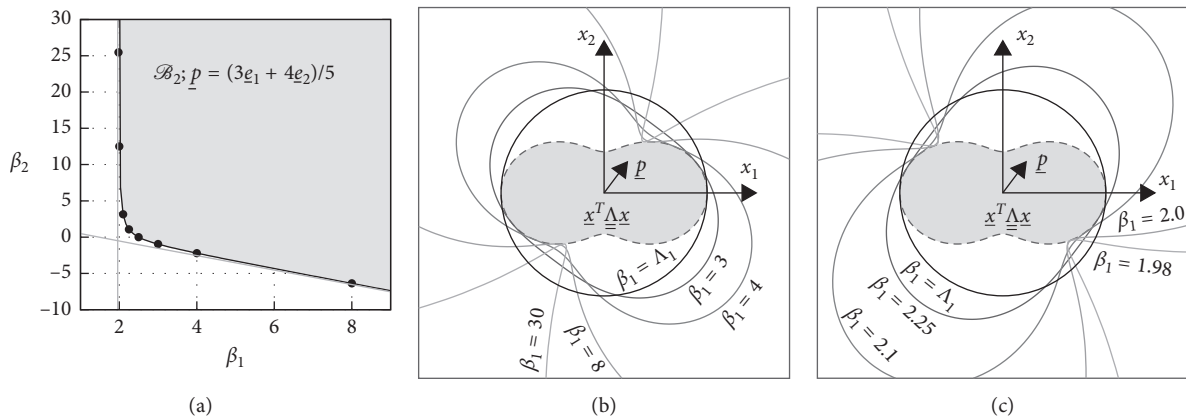


FIGURE 5: (a) Parameter region \mathcal{B}_2 for \underline{A} and \underline{p}_3 ; (b) isolines of the quadratic forms $\underline{x}^T \underline{A} \underline{x}$ and $\underline{x}^T \underline{B}_2 \underline{x}$ in the $(1,2)$ -plane for all normalized \underline{x} for the marked black points of (a) for $\Lambda_1 = 5/2 \leq \beta_1$; (c) evaluation of corresponding points for $\mu_0 < \beta_1 \leq \Lambda_1 = 5/2$.

\underline{B}_2^0 , cf. (8). A short inspection of \underline{B}_4 shows that it may be represented as a rank-two perturbed scaled identity. As in Section 3, we perform a change of basis with the orthogonal matrix

$$\underline{U}_4 = \begin{pmatrix} \underline{U} & \underline{o} \\ \underline{o}^T & 1 \end{pmatrix}, \quad (62)$$

diagonalizing the upper left block of \underline{A}_4 , i.e., we define

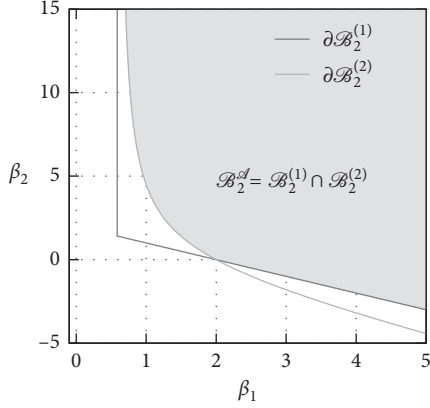


FIGURE 6: The straight lines depict the border of the set $\mathcal{B}_2^{(1)}$, the curved line represents the border of the set $\mathcal{B}_2^{(2)}$, and the gray region illustrates the set \mathcal{B}_2^{ad} .

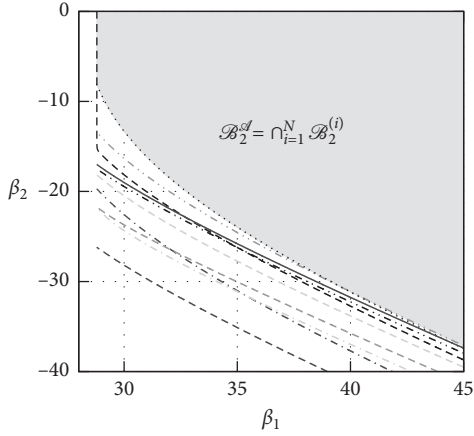


FIGURE 7: The gray region indicates the admissible domain \mathcal{B}_2^{ad} of a set of 10 random matrices of dimension 100. Individual lines represent $\beta_2^{\min}(\beta_1)$ values for each matrix.

$$\underline{\underline{A}}_4 = \underline{U}_4^T \underline{A}_4 \underline{U}_4 = \begin{pmatrix} \underline{A} & \underline{l} \\ \underline{l}^T & l_0 \end{pmatrix}, \quad \underline{l} = \underline{U}_4^T \underline{a}, \quad l_0 = a_0, \quad (63)$$

$$\underline{\underline{B}}_4 = \underline{U}_4^T \underline{B}_4 \underline{U}_4 = \begin{pmatrix} \underline{B}_2 & \beta_4 \underline{p} \\ \beta_4 \underline{p}^T & \beta_3 \end{pmatrix}, \quad \underline{p} = \underline{U}_4^T \underline{p}_0. \quad (64)$$

In this section, $\underline{\underline{B}}_4$ is examined, i.e., we seek the parameter conditions describing the set

$$\mathcal{B}_4 = \{ \underline{\beta} \in \mathbb{R}^4 : \underline{\underline{A}}_4 \leq \underline{\underline{B}}_4 \}. \quad (65)$$

As in Section 3.1, the present section is organized as follows:

- (i) Preparations: introduction of several expressions and relations needed for all the following results
- (ii) Lemma 4: description of \mathcal{B}_4 based on $(\beta_1, \beta_2) \in \partial \mathcal{B}_2$
- (iii) Lemma 5: description of \mathcal{B}_4 based on $(\beta_1, \beta_2) \in \mathcal{B}_2 \setminus \partial \mathcal{B}_2$
- (iv) Corollary 2: recapitulation of the admissible regions for (β_3, β_4) for $(\beta_1, \beta_2) \in \mathcal{B}_2$ and $\mu_\varnothing < \beta_1$ based on the results of Lemma 4 and Lemma 5

- (v) Remark 5: remarks on an additional constraint for a simplification of implementation based on a numerical point of view and Corollary 2

Preparations. For the sake of a compact notation, we define the difference matrix

$$\begin{aligned} \underline{\underline{C}}_4 &= \underline{\underline{B}}_4 - \underline{\underline{A}}_4 = \begin{pmatrix} \underline{C} & \underline{c} \\ \underline{c}^T & c_0 \end{pmatrix}, \\ \underline{C} &= \underline{B}_2 - \underline{A}, \\ \underline{c} &= \beta_4 \underline{p} - \underline{l}, \\ c_0 &= \beta_3 - l_0, \end{aligned} \quad (66)$$

at what positive semidefiniteness of $\underline{\underline{C}}_4$

$$0 \leq \underline{y}^T \underline{\underline{C}}_4 \underline{y} \quad \forall \underline{y} = \begin{pmatrix} \underline{x} \\ x_0 \end{pmatrix} \in \mathbb{R}^{n+1}, \quad (67)$$

is equivalent to $\underline{\underline{A}}_4 \leq \underline{\underline{B}}_4$. More explicitly, (67) can also be expressed as

$$0 \leq \underline{x}^T \underline{C} \underline{x} + 2x_0 \underline{x}^T \underline{c} + c_0 x_0^2, \quad \forall \underline{x} \in \mathbb{R}^n, x_0 \in \mathbb{R}, \quad (68)$$

which allows to obtain the equivalence relation

$$\underline{\underline{O}} \leq \underline{\underline{C}}_4 \iff \underline{\underline{O}} \leq \underline{C} \wedge \underline{c} \perp \ker(\underline{C}) \wedge \underline{c}^T \underline{C}^+ \underline{c} \leq c_0, \quad (69)$$

where \underline{C}^+ denotes the Moore–Penrose inverse of \underline{C} , see, e.g., [25] for a derivation based on the Schur complement. It should be noted that for positive semidefinite \underline{C} , \underline{C}^+ is also positive semidefinite such that c_0 necessarily has to be nonnegative. The condition $\underline{\underline{O}} \leq \underline{\underline{C}}$ is fulfilled for the corresponding $(\beta_1, \beta_2) \in \mathcal{B}_2$ of Section 3. We consider, therefore, the following cases for singular positive semidefinite and positive definite \underline{C} , i.e., based on Section 3, for $(\beta_1, \beta_2) \in \partial \mathcal{B}_2$ and $(\beta_1, \beta_2) \in \mathcal{B}_2 \setminus \partial \mathcal{B}_2$, respectively.

Lemma 4. *If $(\beta_1, \beta_2) \in \partial \mathcal{B}_2$ holds, then the parameter set \mathcal{B}_4 is described by*

$$\begin{aligned} \mathcal{B}_4 &= \left\{ \underline{\beta} \in \mathbb{R}^4 : \right. \\ &(\beta_1, \beta_2) \in \partial \mathcal{B}_2 \wedge (\beta_4 \underline{p} - \underline{l}) \perp \ker(\underline{B}_2 - \underline{A}) \\ &\left. \wedge \beta_3 \geq l_0 + (\beta_4 \underline{p} - \underline{l})^T (\underline{B}_2 - \underline{A})^+ (\beta_4 \underline{p} - \underline{l}) \right\}. \end{aligned} \quad (70)$$

Proof. For a better overview of the following proof, the reader should consider Figure 8 along the following arguments. For $(\beta_1, \beta_2) \in \partial \mathcal{B}_2$, \underline{C} is positive semidefinite and $\det(\underline{C}) = 0$ holds such that the kernel $\ker(\underline{C})$ is nonempty. For sharp majorants $\underline{\underline{B}}_4$ to exist, $\underline{c} \perp \ker(\underline{C})$, cf. (69), describes the critical condition. We notice the following cases:

- (1) $\kappa = 1$: the kernel of \underline{C} is one-dimensional, i.e., $\ker(\underline{C}) = \text{span}\{\underline{n}\}$

(i) In Lemma 1, cf. Remark 1, for

- (a) (28) with $\underline{n} \perp \underline{p}$ (left border without corner of \mathcal{B}_2) or

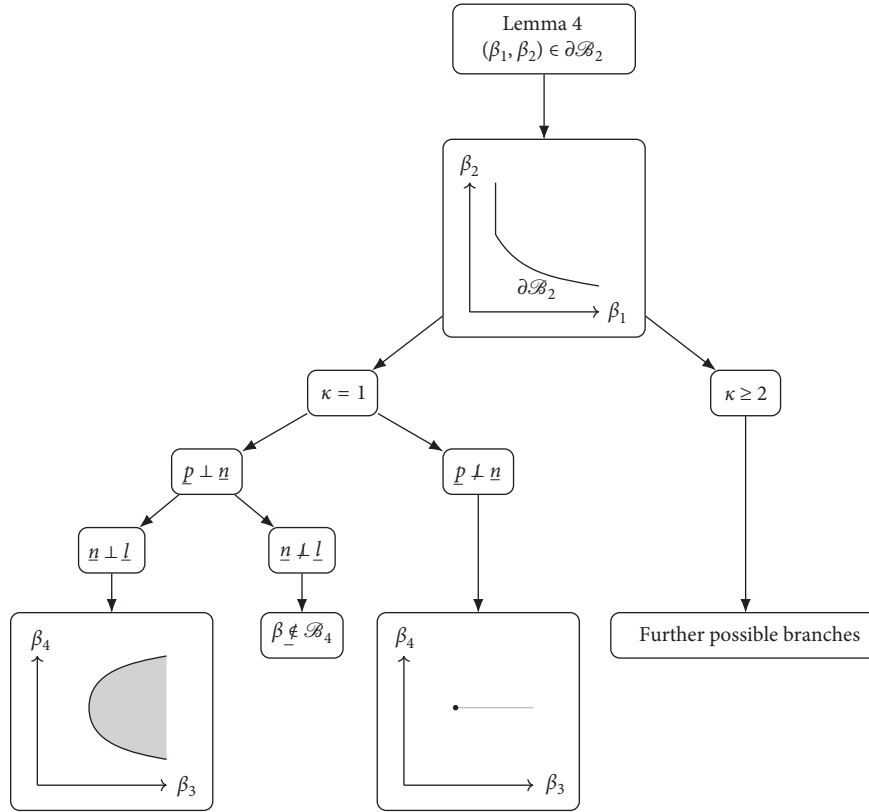


FIGURE 8: Illustration of cases occurring in Lemma 4.

- (b) (29) with $\underline{n} \perp \underline{p}$ (lower border without corner of \mathcal{B}_2)
- (ii) In Lemma 2, cf. Remark 2 and Figure 2, for
 - (a) (45) and (46) with $\underline{n} \perp \underline{p}$ (left border without corner of \mathcal{B}_2 for $\mu_{\mathcal{Q}} = \Lambda_1$),
 - (b) (48) with $\underline{n} \perp \underline{p}$ (left border without corner of \mathcal{B}_2 for $\mu_{\mathcal{Q}} = \Lambda_2 < \Lambda_1$), or
 - (c) (44) and (47) with $\underline{n} \perp \underline{p}$ (lower border without corner of \mathcal{B}_2)
- (iii) In Lemma 3, cf. Remark 3, with $\underline{n} \perp \underline{p}$ on the whole border of \mathcal{B}_2

If $\ker(\underline{C})$ is one-dimensional, for majorants \underline{B}_4 to exist

$$0 = \underline{n}^T \underline{c} = \beta_4 \underline{n}^T \underline{p} - \underline{n}^T \underline{l}, \quad (71)$$

needs to hold, cf. (69). The condition (71) may or may not be fulfilled in a number of exotic cases since some portions of $\partial\mathcal{B}_2$, as, e.g., in (28), have a one-dimensional kernel but with $\underline{p} \perp \underline{n}$.

- (a) If $\underline{p} \perp \underline{n}$ holds, cf. Figure 8, then β_4 loses influence in (71) such that (71) can be fulfilled iff $\underline{n} \perp \underline{l}$ holds, which is not controllable by the parameters β but solely dictated by the given data \underline{A}_4 and \underline{p}_0 , with resulting $\underline{p} = \underline{U}^T \underline{p}_0$ and

$\underline{l} = \underline{U}^T \underline{a}$. If additionally $\underline{n} \perp \underline{l}$ holds, then (71) is fulfilled for all β_4 such that, according to (69), majorants \underline{B}_4 exist if for given $(\beta_1, \beta_2) \in \partial\mathcal{B}_2$, the remaining parameters β_3 and β_4 are chosen such that

$$\begin{aligned} \underline{c}^T \underline{C}^+ \underline{c} &= (\beta_4 \underline{p} - \underline{l})^T (\underline{B}_2 - \underline{\Delta})^+ (\beta_4 \underline{p} - \underline{l}) \\ &\leq c_0 = \beta_3 - l_0, \end{aligned} \quad (72)$$

holds. For instance, the left-hand side term $\underline{c}^T \underline{C}^+ \underline{c}$ of (72) is quadratic in β_4 and is minimized for

$$\frac{\partial \underline{c}^T \underline{C}^+ \underline{c}}{\partial \beta_4} = 2 \underline{p}^T \underline{C}^+ \underline{c} = 0 \implies \beta_4 = \frac{\underline{p}^T \underline{C}^+ \underline{l}}{\underline{p}^T \underline{C}^+ \underline{p}}, \quad (73)$$

which then yields in (72) the lowest possible c_0 and corresponding β_3 , cf. Figure 8. Naturally, if $\underline{n} \perp \underline{l}$ holds, then (71) is not fulfilled and no majorants exist under the current assumptions for $(\beta_1, \beta_2) \in \partial\mathcal{B}_2$, cf. Figure 8.

- (b) If $\underline{p} \perp \underline{n}$ holds, which is the case, e.g., on the lower border of \mathcal{B}_2 in Lemma 1 and Lemma 2 (up to $\beta_1 = \mu_{\mathcal{Q}}$) and on the whole border of \mathcal{B}_2 in Lemma 3, then (71) can be solved uniquely for β_4 , yielding

$$\beta_4 = \frac{\underline{n}^T \underline{l}}{\underline{n}^T \underline{p}}. \quad (74)$$

From (74), one can obtain based on (69), i.e., $c_0 = \beta_3 - l_0 \geq \underline{c}^T \underline{C}^+ \underline{c}$, the minimum β_3

$$\beta_3 \geq l_0 + \left(\frac{\underline{n}^T \underline{l}}{\underline{n}^T \underline{p}} \underline{p} - \underline{l} \right)^T \underline{C}^+ \left(\frac{\underline{n}^T \underline{l}}{\underline{n}^T \underline{p}} \underline{p} - \underline{l} \right), \quad (75)$$

cf. Figure 8.

(2) $\kappa \geq 2$: if the dimension of $\ker(\underline{C})$ is greater than one, then the kernel is described as

$$\ker(\underline{C}) = \text{span}\{\underline{n}_1, \dots, \underline{n}_\kappa\}, \quad (76)$$

at what we choose, without loss of generality, the kernel basis vectors \underline{n}_i such than at maximum only one, say \underline{n}_1 , is not perpendicular to \underline{p} , i.e.,

$$\underline{n}_i^T \underline{p} = 0, \quad \forall i = 2, \dots, \kappa. \quad (77)$$

The condition $\underline{c} \perp \ker(\underline{C})$ is then equivalent to

$$0 = \beta_4 \underline{n}_1^T \underline{p} - \underline{n}_1^T \underline{l} \wedge 0 = \underline{n}_i^T \underline{l}, \quad \forall i = 2, \dots, \kappa. \quad (78)$$

Therefore, (78) makes clear that, for $(\beta_1, \beta_2) \in \partial \mathcal{B}_2$ and $\kappa \geq 2$, the provided data \underline{A}_4 and \underline{p}_0 inducing \underline{p} and \underline{l} decide on the existence of majorants under the current assumptions. If $\underline{l} \perp \underline{n}_i$ for $i = 2, \dots, \kappa$ holds, then the remaining condition $0 = \beta_4 \underline{n}_1^T \underline{p} - \underline{n}_1^T \underline{l}$ in (78) can be analyzed as in case 1, yielding analogous results. \square

Lemma 5. *If $(\beta_1, \beta_2) \in \mathcal{B}_2 \setminus \partial \mathcal{B}_2$ holds, then the parameter set \mathcal{B}_4 is described by*

$$\begin{aligned} \mathcal{B}_4 &= \left\{ \underline{\beta} \in \mathbb{R}^4: \right. \\ &(\beta_1, \beta_2) \in \mathcal{B}_2 \setminus \partial \mathcal{B}_2 \\ &\wedge \beta_3 \geq l_0 + (\beta_4 \underline{p} - \underline{l})^T (\underline{B}_2 - \underline{A})^{-1} (\beta_4 \underline{p} - \underline{l}) \left. \right\}. \end{aligned} \quad (79)$$

Proof. For β_1 and β_2 chosen according to the results of Section 3 truly inside of \mathcal{B}_2 , cf. Figure 9, the difference matrix $\underline{C} = \underline{B}_2 - \underline{A}$ is positive definite. For \underline{C}_4 to be singular, its determinant must vanish. Based on the decomposition

$$\begin{aligned} \underline{C}_4 &= \underline{C}_0 + \underline{U} \underline{V}^T, \quad \underline{C}_0 = \begin{pmatrix} \underline{C} & \underline{o} \\ \underline{o}^T & 1 \end{pmatrix}, \\ \underline{U} &= \begin{pmatrix} \underline{c} & \underline{o} \\ c_0 - 1 & 1 \end{pmatrix}, \underline{V} = \begin{pmatrix} \underline{o} & \underline{c} \\ 1 & 0 \end{pmatrix}, \end{aligned} \quad (80)$$

the matrix determinant lemma yields

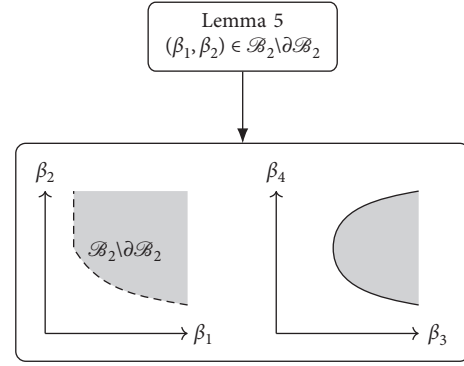


FIGURE 9: Illustration of Lemma 5.

$$\begin{aligned} 0 &= \det(\underline{C}_4) \\ &= \det(\underline{C}_0 + \underline{U} \underline{V}^T) \\ &= \det(\underline{C}_0) \det(\underline{I}_2 + \underline{V}^T \underline{C}_0^{-1} \underline{U}) \\ &= \det(\underline{C}) (c_0 - \underline{c}^T \underline{C}^{-1} \underline{c}), \end{aligned} \quad (81)$$

which, for $c_0 = \beta_3 - l_0$ is fulfilled iff

$$\beta_3 = l_0 + \underline{c}^T \underline{C}^{-1} \underline{c}. \quad (82)$$

This result is in accordance with (69) and delivers a singular positive semidefinite \underline{C}_4 . The parameter β_4 is free and coupled to the minimum β_3 given in (82) through the positive quadratic term $\underline{c}^T \underline{C}^{-1} \underline{c}$, where $\underline{c} = \beta_4 \underline{p} - \underline{l}$, cf. (66). By demanding stationarity of $\underline{c}^T \underline{C}^{-1} \underline{c}$ in respect to β_4 , one obtains

$$\frac{\partial \underline{c}^T \underline{C}^{-1} \underline{c}}{\partial \beta_4} = 2 \underline{p}^T \underline{C}^{-1} \underline{c} = 0 \implies \beta_4 = \frac{\underline{p}^T \underline{C}^{-1} \underline{l}}{\underline{p}^T \underline{C}^{-1} \underline{p}}. \quad (83)$$

Due to the positive definiteness of \underline{C} , the choice (83) $\underline{p}^T \underline{C}^{-1} \underline{c} = 0$ induces a minimum of β_3 in (82):

$$\beta_3 = l_0 + (\beta_4 \underline{p} - \underline{l})^T \underline{C}^{-1} \underline{c} = l_0 - \underline{l}^T \underline{C}^{-1} \underline{c}, \quad (84)$$

cf. Figure 9. \square

Corollary 2. *For any point $(\hat{\beta}_1, \hat{\beta}_2) \in \partial \mathcal{B}_2$ with $\mu_{\mathcal{Q}} < \hat{\beta}_1$, the family of admissible (β_3, β_4) points generated with $(\hat{\beta}_1, \hat{\beta}_2) \in \mathcal{B}_2 \setminus \partial \mathcal{B}_2$ and $\beta_2 > \hat{\beta}_2$ is described by parabolas with common minimum and argument of it. The argument of the minimum of all parabolas is given by the unique admissible value β_4 at $(\hat{\beta}_1, \hat{\beta}_2) \in \partial \mathcal{B}_2$.*

Proof. Consider Figure 10. For any $(\hat{\beta}_1, \hat{\beta}_2) \in \partial \mathcal{B}_2$, e.g., the point depicted in Figure 10 marked with a triangle, based on Remark 1, Remark 2, and Remark 3, we know that, for $\beta_1 > \mu_{\mathcal{Q}}$ on the lower boundary of \mathcal{B}_2 , the relations $\kappa = 1$, $\ker(\underline{C}) = \text{span}\{\underline{n}\}$, $\underline{n} = \underline{D}^{-1} \underline{p}$, and $\underline{n} \perp \underline{p}$ hold. Based on the proof of Lemma 4, admissible (β_3, β_4) are described by the unique admissible $\beta_4^{\text{Lemma 4}}$ given in (74) and inequality (75), cf. the branch for $\kappa = 1$ and $\underline{n} \perp \underline{p}$ in Figure 8. For points $(\hat{\beta}_1, \hat{\beta}_2) \in \mathcal{B}_2 \setminus \partial \mathcal{B}_2$ with $\beta_2 > \hat{\beta}_2$, the corresponding

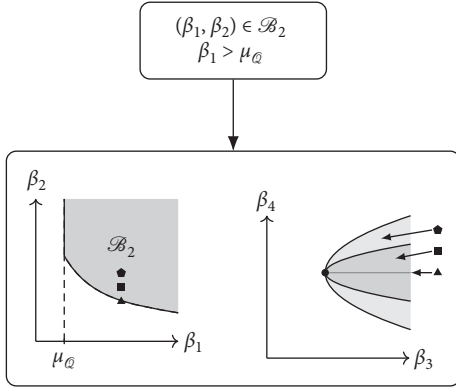


FIGURE 10: Illustration of Corollary 2.

admissible domains for (β_3, β_4) are described through Lemma 5, at what the stationary point of these parabolas is given at $\beta_4^{\text{Lemma 5}}$ fulfilling (83). The unique admissible $\beta_4^{\text{Lemma 4}}$ given in (74) and the stationary point $\beta_4^{\text{Lemma 5}}$ given in (83) are identical for $(\beta_1, \hat{\beta}_2) \in \partial \mathcal{B}_2$ and $(\hat{\beta}_1, \beta_2) \in \mathcal{B}_2 \setminus \partial \mathcal{B}_2$ with $\beta_2 > \hat{\beta}_2$. This is shown as follows. Based on the kernel vector $\underline{n} = \underline{D}^{-1} \underline{p}$ for the regular $\underline{D} = \hat{\beta}_1 \underline{I} - \underline{A}$, the inverse of the difference matrix \underline{C} is expressed with the Sherman–Morrison formula as

$$\begin{aligned} \underline{C}^{-1} &= (\underline{D} + \beta_2 \underline{p} \underline{p}^T)^{-1} = \underline{D}^{-1} - \beta_2 \frac{\underline{D}^{-1} \underline{p} \underline{p}^T \underline{D}^{-1}}{1 + \beta_2 \underline{p}^T \underline{D}^{-1} \underline{p}} \\ &= \underline{D}^{-1} - \beta_2 \frac{\underline{n} \underline{n}^T}{1 + \beta_2 \underline{p}^T \underline{n}}. \end{aligned} \quad (85)$$

It should be emphasized again that, in (85), β_2 is chosen truly in the interior of \mathcal{B}_2 , but \underline{C}^{-1} can always be represented with the kernel vector $\underline{n} = \underline{D}^{-1} \underline{p}$ obtained at $(\hat{\beta}_1, \hat{\beta}_2) \in \partial \mathcal{B}_2$. The relation (85) implies for the stationary point $\beta_4^{\text{Lemma 5}}$ given in (83)

$$\begin{aligned} \beta_4^{\text{Lemma 5}} &= \frac{\underline{l}^T \underline{C}^{-1} \underline{p}}{\underline{p}^T \underline{C}^{-1} \underline{p}} = \frac{\underline{l}^T \underline{n} [1 - \beta_2 (\underline{p}^T \underline{n} / (1 + \beta_2 \underline{p}^T \underline{n}))]}{\underline{p}^T \underline{n} [1 - \beta_2 (\underline{p}^T \underline{n} / (1 + \beta_2 \underline{p}^T \underline{n}))]} \\ &= \frac{\underline{l}^T \underline{n}}{\underline{p}^T \underline{n}} = \beta_4^{\text{Lemma 4}}, \end{aligned} \quad (86)$$

such that $\beta_4^{\text{Lemma 4}}$, cf. (74), and $\beta_4^{\text{Lemma 5}}$ are identical, as depicted in Figure 10. The corresponding values of the minima $\beta_3^{\text{Lemma 5}} = l_0 - \underline{l}^T \underline{C}^{-1} \underline{c}$ given in (84) of the parabolas are identical to the minimum $\beta_3^{\text{Lemma 4}} = l_0 + \underline{c}^T \underline{C}^+ \underline{c}$ of (75). This is shown as follows. First, the minimum of the parabolas $\beta_3^{\text{Lemma 5}} = l_0 - \underline{l}^T \underline{C}^{-1} \underline{c}$ requires the computation of $\underline{C}^{-1} \underline{c}$. Hereby, it is useful to note that since $\beta_4^{\text{Lemma 4}} = \beta_4^{\text{Lemma 5}}$ holds, the vector $\underline{c} = \beta_4^{\text{Lemma 5}} \underline{p} - \underline{l} = \beta_4^{\text{Lemma 4}} \underline{p} - \underline{l}$ is orthogonal to \underline{n} , i.e., $\underline{c}^T \underline{n} = 0$, cf. (71) corresponding to Lemma 4. Based on the Sherman–Morrison

formula for \underline{C}^{-1} (85) and the property $\underline{c} \perp \underline{n}$, the minimum $\beta_3^{\text{Lemma 5}}$, cf. (84), is simplified as follows:

$$\beta_3^{\text{Lemma 5}} = l_0 - \underline{l}^T \underline{C}^{-1} \underline{c} = l_0 - \underline{l}^T \underline{D}^{-1} \underline{c}. \quad (87)$$

Now, concerning the minimum $\beta_3^{\text{Lemma 4}} = l_0 + \underline{c}^T \underline{C}^+ \underline{c}$ for $(\hat{\beta}_1, \hat{\beta}_2) \in \partial \mathcal{B}_2$ and $\beta_4^{\text{Lemma 4}}$, cf. (75), the Moore–Penrose inverse $\underline{C}^+ = (\underline{D} + \beta_2 \underline{p} \underline{p}^T)^+$ is required. Based on [26] (cf. Theorem 6 therein), \underline{C}^+ can be expressed as

$$(\underline{D} + \beta_2 \underline{p} \underline{p}^T)^+ = \underline{D}^{-1} - \frac{1}{\underline{n}^T \underline{n}} (\underline{n} \underline{n}^T \underline{D}^{-1} + \underline{D}^{-1} \underline{n} \underline{n}^T - (\underline{n}^T \underline{p}) \underline{n} \underline{n}^T). \quad (88)$$

Consideration of $\underline{c} \perp \underline{n}$, cf. Lemma 4, yields

$$\begin{aligned} \beta_3^{\text{Lemma 4}} &= l_0 + \underline{c}^T \underline{C}^+ \underline{c} = l_0 + \underline{c}^T \underline{D}^{-1} \underline{c} \\ &= l_0 + \underline{c}^T (\beta_4^{\text{Lemma 4}} \underline{n} - \underline{D}^{-1} \underline{l}) = l_0 - \underline{l}^T \underline{D}^{-1} \underline{c}, \end{aligned} \quad (89)$$

such that the minima of the parabolas (87) and (89) are identical, as depicted in Figure 10. \square

Remark 5. It should be noted that in view of future optimization problems over \mathcal{B}_4 , from a numerical point of view, all tedious cases on the left border of \mathcal{B}_2 with $\mathcal{P} \perp \ker(\underline{C})$ and $\kappa \geq 2$ for Lemma 1 and Lemma 2 can be avoided easily. This is achieved through Corollary 2 and by imposing the additional constraint

$$\mu_Q^s \leq \beta_1, \quad \mu_Q^s = \mu_Q + \delta, \quad 0 < \delta \ll 1, \quad (90)$$

in standard numerical optimization procedures as a limit constraint for β_1 with a shifted constant μ_Q^s slightly greater than μ_Q for some user-defined δ . The shifted condition (90) and Corollary 2 allow for a straightforward and simple implementation of the corresponding results of Lemma 4 and Lemma 5. This approach has been considered for the implementation offered in [22].

4.2. Majorization of a Set of Matrices. As in the two-parametric case, for a given vector $\underline{p}_0 \in \mathbb{R}^n$ and a given matrix set

$$\mathcal{A} = \{\underline{A}_4^{(1)}, \dots, \underline{A}_4^{(N)}\}, \quad \underline{A}_4 \in \mathcal{S}_{n+1} \forall \underline{A}_4 \in \mathcal{A}, \quad (91)$$

with as in (60) partitioned matrices, we define the sets

$$\mathcal{B}_4^{(i)} = \{\underline{\beta} \in \mathbb{R}^4 : \underline{A}_4^{(i)} \leq \underline{B}_4^0\}. \quad (92)$$

The majorant set of \mathcal{A} is the corresponding intersection of all $\mathcal{B}_4^{(i)}$:

$$\mathcal{B}_4^{\mathcal{A}} = \bigcap_{i=1}^N \mathcal{B}_4^{(i)}. \quad (93)$$

5. Application to Semidefinite Programming

For a given finite matrix set

$$\mathcal{A} = \{\underline{A}^{(1)}, \dots, \underline{A}^{(N)}\}, \quad \underline{A} \in \mathcal{S}_v \forall \underline{A} \in \mathcal{A}, \quad (94)$$

consider the majorant set $\mathcal{B}_d^{\mathcal{A}}$ of \mathcal{A} for some parametrized $\underline{B}(\underline{\beta}) \in \mathcal{S}$, with parameter vector $\underline{\beta} \in \mathbb{R}^d$

$$\mathcal{B}_d^{\mathcal{A}} = \{ \underline{\beta} \in \mathbb{R}^d : \underline{A} \preceq \underline{B}(\underline{\beta}) \forall \underline{A} \in \mathcal{A} \}. \quad (95)$$

The objective is now the minimization of a function $\varphi: \mathbb{R}^d \mapsto \mathbb{R}$ over $\mathcal{B}_d^{\mathcal{A}}$:

$$\min_{\underline{\beta} \in \mathcal{B}_d^{\mathcal{A}}} \varphi(\underline{\beta}). \quad (96)$$

If the function $\underline{B}(\underline{\beta})$ is linear in the parameter $\underline{\beta}$, which is assumed from this point on, then $\mathcal{B}_d^{\mathcal{A}}$ is nonempty, unbounded, and convex, and the minimization problem (96) is a classical semidefinite programming problem (see, e.g., [7]) such that it may be tackled with several numerical approaches from literature (see, e.g., [8, 10, 12]). For continuous and convex φ , the minimum, if it exists, may be located in the interior of $\mathcal{B}_d^{\mathcal{A}}$ or on its border $\partial\mathcal{B}_d^{\mathcal{A}}$. Therefore, an unconstrained optimization should always be performed first. If its solution is not an element of the interior of $\mathcal{B}_d^{\mathcal{A}}$, then a constrained optimization problem may be considered to find the optimum on $\partial\mathcal{B}_d^{\mathcal{A}}$, i.e., among the sharp Löwner majorants. It should be remarked that convex functions φ can be formulated for corresponding convex $\mathcal{B}_d^{\mathcal{A}}$ such that no minimum exists. A clear example for such a case is constructed based on the results of Section 3 for a single matrix. Assume the two-parametric form $\underline{B} = \underline{B}_2^0$ of Section 3 and choose $\underline{A} = \underline{A}^{(2)}$ and \underline{p}_0 as given in (58) and (59) such that \underline{p}_0 is not an eigenvector of \underline{A} and $\Lambda_2 < \mu_{\mathcal{Q}} < \Lambda_2$ holds. This implies an instance of Lemma 3, yielding the region $\mathcal{B}_d^{\mathcal{A}} = \mathcal{B}_2$ as depicted in Figure 6 for $\mathcal{B}_2^{(2)}$. Now, consider the linear function $\varphi(\underline{\beta}) = \underline{g}^T \underline{\beta}$ with constant gradient $\underline{g} \in \mathbb{R}^2$. An example is displayed in Figure 11(a) with $\underline{g} = (3, 1)^T$.

Regarding Figure 11(a), it becomes immediately clear that a minimum of the convex $\varphi(\underline{\beta})$ exists in the current \mathcal{B}_2 . But, this is not always the case for arbitrary \underline{g} since, e.g., for $\underline{g} = (0, 1)^T$ values on the lower boundary of \mathcal{B}_2 continuously decrease due to the unboundedness of \mathcal{B}_2 emphasized in Corollary 1 such that no minimum exists for $\underline{g} = (0, 1)^T$. Therefore, in general, depending on the properties of the convex set $\mathcal{B}_d^{\mathcal{A}}$ and on the properties of the convex $\varphi(\underline{\beta})$, a minimum may exist. For the rest of this section, we do not consider such cases, i.e., we assume that the convex $\varphi(\underline{\beta})$ is formulated such that a global minimum exists in $\mathcal{B}_d^{\mathcal{A}}$, as in the examples shown in Figure 11. These examples can be reproduced with

demo3.m

in [22]. The global minimum for instances of Lemma 3, as the examples depicted in Figure 11, is obtained by solving the single nonlinear equation for β_1

$$\begin{aligned} \underline{g}^T \underline{t}|_{\beta_2 = \beta_2^{\min}(\beta_1)} &= 0, \\ \underline{g} &= \left(\frac{\partial \varphi}{\partial \beta_1}, \frac{\partial \varphi}{\partial \beta_2} \right)^T, \\ \underline{t} &= \left(1, \frac{\partial \beta_2^{\min}}{\partial \beta_1} \right)^T, \end{aligned} \quad (97)$$

based on the orthogonality of the gradient \underline{g} of φ and the tangent \underline{t} of the curve $(\beta_1, \beta_2^{\min})$ for $\beta_1 > \mu_{\mathcal{Q}}$. An initial guess can be generated with the trivial majorant, i.e., $\beta_1 = \Lambda_1$, such that standard numerical approaches solving the nonlinear equation for β_1 can be used, independently of the dimension of the given matrix \underline{A} .

As mentioned in Section 1, the presented results can also be used in the context of the zeroth-order bounds of elasticity. The upper zeroth-order bound of, e.g., graphite, see [16], with stiffness matrix given in GPa (10^9N/m^2) in normalized Voigt notation, see, e.g., [27],

$$\underline{A} = \begin{pmatrix} 1060 & 180 & 15 & 0 & 0 & 0 \\ 180 & 1060 & 15 & 0 & 0 & 0 \\ 15 & 15 & \frac{73}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 9 & 0 & 0 \\ 0 & 0 & 0 & 0 & 9 & 0 \\ 0 & 0 & 0 & 0 & 0 & 880 \end{pmatrix} \text{GPa} \in \mathbb{R}^{6 \times 6}, \quad (98)$$

and dimensionless vector \underline{p}_0 given by

$$\underline{p}_0 = (1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3}, 0, 0, 0) \in \mathbb{R}^6, \quad (99)$$

were defined in [16] through the minimization of $\varphi = \text{tr}(\underline{B}_2^0) = 6\beta_1 + \beta_2$, where β_1 and β_2 are also given in GPa. In engineering, the bulk modulus K and the shear modulus G are related to β_1 and β_2 by $K = (\beta_1 + \beta_2)/3$ and $G = \beta_1/2$. The case for graphite yields

$$\begin{aligned} &\{\Lambda_1, \Lambda_2, \Lambda_3, \Lambda_4, \Lambda_5, \Lambda_6\} \\ &= \left\{ \frac{1}{4} (\sqrt{5800849} + 2553), 880, 880, \right. \\ &\quad \left. \frac{1}{4} (2553 - \sqrt{5800849}), 9, 9 \right\} \text{GPa}, \end{aligned} \quad (100)$$

$$\mu_{\mathcal{Q}} = 880 \text{GPa}, \quad c_{\mathcal{Q}} = -\frac{1387}{912330} \frac{1}{\text{GPa}},$$

i.e., an instance of Lemma 2.2. This shows that, in general, Lemma 2.1 and Lemma 2.2 are also relevant for real-world

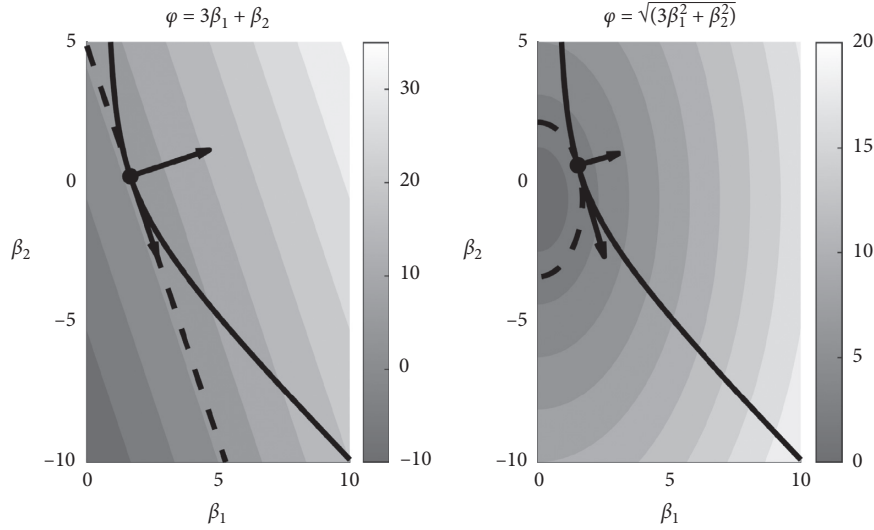


FIGURE 11: Examples for linear and nonlinear function φ over \mathcal{B}_2 : $\varphi = 3\beta_1 + \beta_2$ (a); $\varphi = \sqrt{3\beta_1^2 + \beta_2^2}$ (b). The gradient of φ and the tangent of the curve $(\beta_1, \beta_2^{\min}(\beta_1))$ at the global minimum (black point) are depicted by the corresponding black arrows, while the dashed line represents $\varphi(\underline{\beta}) = \min_{\beta \in \mathcal{B}_2} \varphi$.

problems and practical applications. In Lemma 2.2, $\beta_1 \in [\mu_{\mathcal{Q}}, \infty)$ is considered, and the corner point $(\beta_1, \beta_2) = (\mu_{\mathcal{Q}}, -(c_{\mathcal{Q}})^{-1}) \in \partial \mathcal{B}_2$ yields the global minimum for φ , see Figure 12. This result is the exact same upper zeroth-order bound of graphite computed by [16] (cf. Table 3 of [16], based on the relations for the bulk modulus $K = (\beta_1 + \beta_2)/3 = 2132890/4161 \text{ GPa} \approx 512.591 \text{ GPa}$ and shear modulus $G = \beta_1/2 = 440 \text{ GPa}$). Compared to [16] and the later development by [17, 19], the present work does not require special treatment for the computation of the minimum of φ over \mathcal{B}_2 since the condensed explicit conditions describing $\partial \mathcal{B}_2$ are now available for evaluation.

The results of the present work may also be applied to more complex semidefinite programming problems in higher dimensions as follows. For a given vector $\underline{p}_0 \in \mathbb{R}^n$, either the case for $\mathcal{S}_v = \mathcal{S}_n$ in (94) with

$$\underline{\underline{B}} = \underline{\underline{B}}_2^0 \implies \mathcal{B}_d^{\mathcal{A}} = \mathcal{B}_2^{\mathcal{A}}, \quad (101)$$

or the case $\mathcal{S}_v = \mathcal{S}_{n+1}$ with

$$\underline{\underline{B}} = \underline{\underline{B}}_4^0 \implies \mathcal{B}_d^{\mathcal{A}} = \mathcal{B}_4^{\mathcal{A}}, \quad (102)$$

can be considered. For (101), minimizers on the border of the convex set $\mathcal{B}_d^{\mathcal{A}} = \mathcal{B}_2^{\mathcal{A}}$ can be determined without much effort based on the results of Section 3. For (102), minimizers can be searched based on the results presented in Section 4. The definition of the majorant of a set of symmetric matrices is nontrivial in the four-parametric version. First, the set $\mathcal{B}_d^{\mathcal{A}}$ should be identified. Then, three options exist: (i) pick critical $(\beta_1, \beta_2) \in \partial \mathcal{B}_2^{\mathcal{A}}$ and choose β_4 carefully (see Lemma 4) or (ii) select subcritical $(\beta_1, \beta_2) \in \mathcal{B}_2^{\mathcal{A}} \setminus \partial \mathcal{B}_2^{\mathcal{A}}$ leading to unconstrained $\beta_4 \in \mathbb{R}$ and β_3 constrained by the lower estimate (82) (see Lemma 5). These constraints can be put into two scalar equations which allow for efficient implementation and fast numerical treatment (see the following examples and accompanying open-source software).

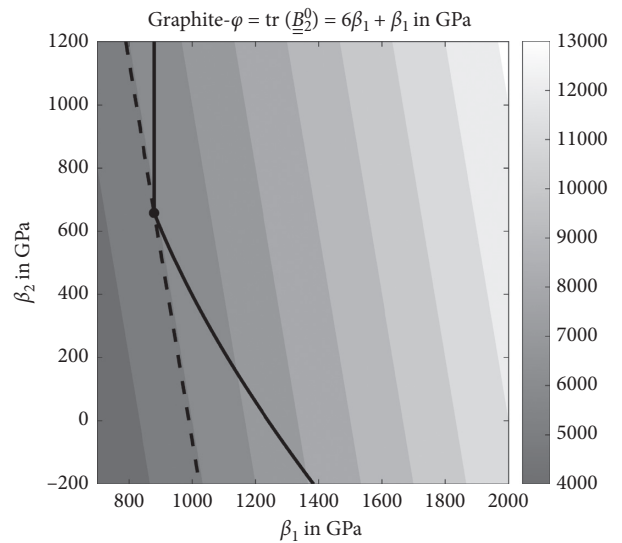


FIGURE 12: Computation of upper zeroth-order bound of [16] based on $\varphi = \text{tr}(\underline{\underline{B}}_2^0) = 6\beta_1 + \beta_1$ for graphite (instance of Lemma 2.2): $\partial \mathcal{B}_2$ (black line), minimum of φ over \mathcal{B}_2 at $(\beta_1, \beta_2) = (\mu_{\mathcal{Q}}, -(c_{\mathcal{Q}})^{-1}) \in \partial \mathcal{B}_2$ (black point), and $\varphi = \min_{(\beta_1, \beta_2) \in \mathcal{B}_2} \varphi$ (dashed lined).

5.1. Example: Four-Parametric Optimization Majorizing a Single Matrix. We consider the semidefinite programming problem (96) for a single matrix $\underline{\underline{A}}_4$ and the four-parametric form $\underline{\underline{B}}_4$ of Section 4. A matrix $\underline{\underline{A}}_4 \in \mathcal{S}_{11}$ and a vector $\underline{p}_0 \in \mathbb{R}^{10}$ with $\Lambda_{11} \approx -11.3075$, $\Lambda_1 \approx 4.7144$, and $\mu_{\mathcal{Q}} \approx 4.206$ are considered in order to optimize the Frobenius norm

$$\varphi(\underline{\beta}) = \|\underline{\underline{B}}_4(\underline{\beta})\|_F = \sqrt{n\beta_1^2 + \beta_2^2 + \beta_3^2 + 2\beta_4^2}, \quad n = 10. \quad (103)$$

Note that the unconstrained minimum of this function is obtained at $\underline{\beta} = \underline{0} \notin \mathcal{B}_4$. Hence, the constrained minimum

will be found on the boundary $\partial\mathcal{B}_4$. The explicit data of the current problem can recovered based on

demo4.m

in the provided software [22].

The results of Lemma 1–Lemma 4 for the explicit construction of sharp majorants may be applied as follows for the generation of an initial guess for the future optimization over \mathcal{B}_4 for a single matrix:

- (1) Generate a discrete point set I_1^h from the interval $I_1 = [\mu_\otimes^s, \beta_1^{\max}]$ with μ_\otimes^s as in (90) (e.g., through an equidistant discretization of I_1)
- (2) Compute the corresponding $\tilde{\beta}_2(\beta_1) = \beta_2^{\min}(\beta_1)$ for each $\beta_1 \in I_1^h$
- (3) Use Lemma 4 noting $\kappa = 1 \wedge \mathcal{P} \perp \ker(\underline{\underline{C}}) \forall \beta_1 \in I_1^h$:
 - (a) Compute the corresponding $\tilde{\beta}_4(\beta_1) = \beta_4(\beta_1, \tilde{\beta}_2(\beta_1))$ with (74)
 - (b) Compute the corresponding $\tilde{\beta}_3(\beta_1) = \text{minimum } \beta_3$ in (75)
- (4) Evaluate objective function $\tilde{\varphi}(\beta_1) = \varphi(\tilde{\beta}(\beta_1))$ accordingly, and return critical β_1^c yielding the minimum value for $\beta_1 \in I_1^h$

Execution of the just described simple approach yields a critical $\beta_1^c = 4.6028$ implying

$$\begin{aligned} \underline{\beta}^c &= (4.6028, -4.1089, 4.5598, -2.4422) \in \partial\mathcal{B}_4, \\ \tilde{\varphi}(\beta_1^c) &= \varphi(\underline{\beta}^c) = 16.1697. \end{aligned} \tag{104}$$

The straightforward implementation of the results of Lemma 4 and Lemma 5 simplified through the additional constraint of Remark 5 yields for the numerical minimization

$$\begin{aligned} \underline{\beta}^* &= (4.6302, 0.3030, 4.6269, -1.1840) \in \partial\mathcal{B}_4, \\ \varphi(\underline{\beta}^*) &= 15.4495 < \varphi(\underline{\beta}^c). \end{aligned} \tag{105}$$

Notably, $\underline{\beta}^c$ induces two zero eigenvalues in $\underline{\underline{C}}_4$, while $\underline{\beta}^*$ leads to a one-dimensional kernel. Algorithmically, the optimization gets away with two nonlinear inequality constraints independently of the dimension n of the problem, see

demo4.m

in [22] for details and reproduction of the results of this example.

5.2. Example: Four-Parametric Optimizations Majorizing a Set of Matrices. Next, we consider the semidefinite programming problem (96) for a finite matrix set $\mathcal{A} = \{\underline{\underline{A}}_4^{(1)}, \dots, \underline{\underline{A}}_4^{(N)}\}$ with $N = 5$ and $n = 10$, $\underline{\underline{B}}_4$ and the Frobenius norm given in (103). The explicit data of the current problem can be recovered based on

demo5.m

in the provided software [22].

The results of Lemma 1–Lemma 5 for the explicit construction of sharp majorants may be used in order to generate an initial guess as follows:

- (1) Generate a discrete point set I_1^h from the interval $I_1 = [\mu_\otimes^s, \beta_1^{\max}]$ with $\mu_\otimes^s > \max_{i=1, \dots, N} \{\mu_\otimes\}$ corresponding to $\underline{\underline{A}}_4^{(i)}$ (e.g., through an equidistant discretization of I_1)
- (2) Compute $\tilde{\beta}_2(\beta_1) = \max_{i=1, \dots, N} \{\beta_2^{\min}(\beta_1)\}$ corresponding to $\underline{\underline{A}}_4^{(i)}$ for $\beta_1 \in I_1^h$ and build discretized curve $\mathcal{C} = \{(\beta_1, \beta_2) \in \mathcal{B}_2^{\mathcal{A}} : \beta_1 \in I_1^h, \beta_2 = \tilde{\beta}_2(\beta_1)\}$
- (3) Shift \mathcal{C} by some small positive Δ into the interior of $\mathcal{B}_2^{\mathcal{A}}$ and rewrite $\mathcal{C} = \{(\beta_1, \beta_2) \in \mathcal{B}_2^{\mathcal{A}} \setminus \partial\mathcal{B}_2^{\mathcal{A}} : (\beta_1, \beta_2) = (\beta_1' + \Delta, \beta_2' + \Delta), (\beta_1', \beta_2') \in \mathcal{C}\}$
- (4) Use Lemma 5:
 - (a) Set $\tilde{\beta}_4(\beta_1) = 0 \forall \beta_1 \in I_1^h$
 - (b) Compute corresponding $\tilde{\beta}_3(\beta_1) = \max_{i=1, \dots, N} \{\beta_3\}$ according to (82) for $\underline{\underline{A}}_4^{(i)}$ with $(\beta_1, \beta_2) \in \mathcal{C}$
- (5) Evaluate $\varphi((\beta_1, \tilde{\beta}_2(\beta_1), \tilde{\beta}_3(\beta_1), \tilde{\beta}_4(\beta_1)))$ for all $\beta_1 \in I_1^h$ and determine minimum
- (6) Go to 3 (i.e., shift \mathcal{C} again by Δ), execute 4 and 5, and if the new minimum is lower, repeat 3–5; otherwise, return minimum

Execution of this simple approach yields for the considered data, the critical value $\beta_1^c = 8.2100$, and accordingly,

$$\underline{\beta}^c = (8.2100, 1.9358, 3.8857, 0), \quad \varphi(\underline{\beta}^c) = 26.3229. \tag{106}$$

The straightforward implementation of the results of Lemma 4 and Lemma 5 simplified through the additional constraint

$$\mu_\otimes^s \leq \beta_1, \quad \mu_\otimes^s = \delta + \max_{i=1, \dots, N} \{\mu_\otimes \text{ corresponding to } \underline{\underline{A}}_4^{(i)}\}, \tag{107}$$

as motivated in Remark 5, yields the minimum of the numerical minimization

$$\begin{aligned} \underline{\beta}^* &= (7.3810, 0.7335, 6.5763, -2.1962), \\ \varphi(\underline{\beta}^*) &= 24.4586 < \varphi(\underline{\beta}^c). \end{aligned} \tag{108}$$

Both β^c and β^* yielded a difference matrix $\underline{\underline{C}}$ with only one vanishing eigenvalue. As in the previous example, the optimization gets away with two nonlinear inequality constraints per matrix $\underline{\underline{A}} \in \mathcal{A}$ independently of the dimension n of the matrices $\underline{\underline{A}} \in \mathcal{A}$, see

demo5.m

in [22] for details and reproduction of the results of this example.

6. Conclusions

Closed form expressions for the representation of two-parametric Löwner majorants based on a rank-one perturbed scaled identity matrix are presented in Section 3. Different scenarios accounting for the multiplicity of eigenvalues and for the inclination of the vector p with respect to the eigenbasis of the matrix under consideration are formulated. The majorization of a set of symmetric matrices \mathcal{A} , yielding the global majorant set $\mathcal{B}_2^{\mathcal{A}}$, is then obtained by an intersection of the individual admissibility domains. Most importantly, the intersection is always unbounded, and thus, nonempty. Analogous results are obtained for the four-parametric case illustrated in Section 4, at what the explicit conditions defining the majorant set, with β_3 and β_4 chosen accordingly, allow for efficient algorithms, cf. Corollary 2 and Remark 5. Examples have been presented for the two- and four-parametric cases. The application of these results in semidefinite programming problems has been sketched in Section 5. The results of the present work also find application in materials science and engineering in the field of materials design of linear elastic and linear thermo-elastic properties. So-called zeroth-order bounds of linear material properties are determined through optimization problems as the one described in Section 5, see, e.g., [17] or [19], such that the results of the present work substantially simplify the computation of the zeroth-order bounds and the related automated selection of material of large material databases. The data and the software for reproduction of the results are available via GitHub, see [22].

Data Availability

Open-source MATLAB software is provided under the terms of the GNU GPL v3. The software is made available through GitHub, cf. [22].

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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