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On the sensitivities of multiple eigenvalues

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Abstract We consider the generalized symmetric eigenvalue problem where matrices depend smoothly on a parameter. It is well known that in general individual eigenvalues, when sorted in accordance with the usual ordering on the real line, do not depend smoothly on the parameter. Nevertheless, symmetric polynomials of a number of eigenvalues, regardless of their multiplicity, which are known to be isolated from the rest depend smoothly on the parameter. We present explicit readily computable expressions for their first derivatives. Finally, we demonstrate the utility of our approach on a problem of finding a shape of a vibrating membrane with a smallest perimeter and with prescribed four lowest eigenvalues, only two of which have algebraic multiplicity one.

Keywords multiple eigenvalues, sensitivity analysis

1 Introduction

Consider a function $\mathbf{A} : \mathbb{R} \to \mathbb{S}^2$ mapping a parameter t into a set of 2×2 symmetric matrices. Even when entries $a_{ij}(t)$, $i, j = 1,2$ depend smoothly on the parameter, the eigenvalues $\lambda_1(t) \le \lambda_2(t)$ may be non-smooth functions at points where their multiplicity changes. Nevertheless, both their sum $\lambda_1(t)+\lambda_2(t) = \operatorname{tr}\mathbf{A}(t) = a_{11}(t)+a_{22}(t)$ and their product $\lambda_1(t)\,\lambda_2(t) = \det\mathbf{A}(t) = a_{11}(t)\,a_{22}(t) - a_{12}(t)\,a_{21}(t)$ clearly remain smooth functions. This knowledge may be used to, for example, replace potentially non-smooth pair of constraints $\lambda_1(t) = \hat\lambda_1$, $\lambda_2(t) = \hat\lambda_2$, with a pair of smooth ones: $\operatorname{tr}\mathbf{A}(t) = \hat\lambda_1 + \hat\lambda_2$, $\det\mathbf{A}(t) = \hat\lambda_1\,\hat\lambda_2$, see [4].

For 2×2 matrices explicit expressions for $[\operatorname{tr}\mathbf{A}(t)]'$ and $[\det\mathbf{A}(t)]'$, where with prime throughout the paper we denote differentiation with respect to t, may be easily obtained in terms of $a_{ij}(t)$, $i, j = 1,2$, and their derivatives. However, we seek an alternative representation of these quantities, which remain valid for higher-dimensional problems. To this end, let $\mathbf{u}_1 : \mathbb{R} \to \mathbb{R}^2$, $\mathbf{u}_2 : \mathbb{R} \to \mathbb{R}^2$ be the normalized eigenvectors corresponding to $\lambda_1(t)$, $\lambda_2(t)$. We assume a computationally realistic situation, when the vectors $\mathbf{u}_1(t)$ and $\mathbf{u}_2(t)$ are *not necessarily continuous* for $t\in\mathbb{R}$ such that $\lambda_1(t) = \lambda_2(t)$. (Indeed, in our simple two-dimensional example an *arbitrary* pair of non-zero vectors $\mathbf{u}_1(t)$ and $\mathbf{u}_2(t)$ constitutes a pair of eigenvectors for $t\in\mathbb{R}$ such that $\lambda_1(t) = \lambda_2(t)$.) However, we do assume that these vectors are chosen to be orthonormal for all $t\in\mathbb{R}$. Whenever the function $\lambda_i(t)$, $i = 1,2$, is differentiable at a point $t_0\in\mathbb{R}$, its derivative is known to satisfy the equation $\lambda_i'(t_0) = \mathbf{u}_i^{\mathrm{T}}(t_0)\mathbf{A}'(t_0)\mathbf{u}_i(t_0)$, $i = 1,2$, see for example [1]. As a result, we get

$$
\begin{aligned}
[\operatorname{tr}\mathbf{A}(t_0)]' &= \sum_{i=1}^{2} \mathbf{u}_i^{\mathrm{T}}(t_0)\mathbf{A}'(t_0)\mathbf{u}_i(t_0),\\
[\det\mathbf{A}(t_0)]' &= \sum_{i=1}^{2} \mathbf{u}_i^{\mathrm{T}}(t_0)\mathbf{A}'(t_0)\mathbf{u}_i(t_0)\prod_{j\ne i}\lambda_j(t_0).
\end{aligned}
\tag{1}
$$

Interestingly enough, these formulas remain valid even when the eigenvalues are not smooth any longer, as well as in higher-dimensional cases. We start by illustrating this phenomenon on a concrete 2×2 example and then proceed to present a general theory.

Example 1 Consider the symmetric 2×2 symmetric matrix

$$
\mathbf{A}(t) = \begin{pmatrix} \cos(t) & \sin(t) \\ \sin(t) & \cos(t) \end{pmatrix}.
$$

Its eigenvalues are

$$
\lambda_1(t) = \cos(t) - |\sin(t)|,
$$
$$
\lambda_2(t) = \cos(t) + |\sin(t)|,
$$

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which are smooth functions of $t \in \mathbb{R}$ except at points $t_k = \pi k$, $k = 0, \pm 1, \pm 2, \ldots$. The corresponding eigenvectors are

$$\mathbf{u}_1(t) = 2^{-1/2}(-|\sin(t)|/\sin(t), 1)^{\mathrm{T}},$$
$$\mathbf{u}_2(t) = 2^{-1/2}(|\sin(t)|/\sin(t), 1)^{\mathrm{T}},$$

for $t \neq t_k$, and an arbitrary pair of orthonormal vectors for $t = t_k$, $k = 0, \pm 1, \pm 2, \ldots$. A direct computation shows that

$$\operatorname{tr}\mathbf{A}(t) = 2\cos(t), \qquad \det\mathbf{A}(t) = \cos(2t),$$
$$[\operatorname{tr}\mathbf{A}(t)]' = -2\sin(t), \qquad [\det\mathbf{A}(t)]' = -2\sin(2t).$$

For $t \neq t_k$, $k = 0, \pm 1, \pm 2, \ldots$, we have

$$\mathbf{u}_1^{\mathrm{T}}(t)\mathbf{A}'(t)\mathbf{u}_1(t) + \mathbf{u}_2^{\mathrm{T}}(t)\mathbf{A}'(t)\mathbf{u}_2(t) = -2\sin(t),$$
$$\lambda_1(t)\mathbf{u}_2^{\mathrm{T}}(t)\mathbf{A}'(t)\mathbf{u}_2(t) + \lambda_2(t)\mathbf{u}_1^{\mathrm{T}}(t)\mathbf{A}'(t)\mathbf{u}_1(t) = -2\sin(2t).$$

Finally, when $t = t_k$ we can for example put

$$\mathbf{u}_1(t_k) = (\sin(\phi), \cos(\phi))^{\mathrm{T}},$$
$$\mathbf{u}_2(t_k) = (\cos(\phi), -\sin(\phi))^{\mathrm{T}},$$

$\phi \in [0, 2\pi)$. Then

$$\mathbf{u}_1^{\mathrm{T}}(t_k)\mathbf{A}'(t_k)\mathbf{u}_1(t_k) + \mathbf{u}_2^{\mathrm{T}}(t_k)\mathbf{A}'(t_k)\mathbf{u}_2(t_k) = 0,$$

as well as

$$\lambda_1(t_k)\mathbf{u}_2^{\mathrm{T}}(t_k)\mathbf{A}'(t_k)\mathbf{u}_2(t_k) + \lambda_2(t_k)\mathbf{u}_1^{\mathrm{T}}(t_k)\mathbf{A}'(t_k)\mathbf{u}_1(t_k) = 0,$$

which is consistent with (1).

Remark 1 Theoretically, for symmetric matrices it is always possible to choose eigenvalue branches, which depend on the parameter in a differentiable manner [2]. In our Example 1 we can of course choose

$$\widetilde{\lambda}_1(t) = \cos(t) - \sin(t),$$
$$\widetilde{\lambda}_2(t) = \cos(t) + \sin(t),$$

which are smooth functions of $t \in \mathbb{R}$ with the corresponding smooth eigenvectors

$$\widetilde{\mathbf{u}}_1(t) = 2^{-1/2}(-1, 1)^{\mathrm{T}},$$
$$\widetilde{\mathbf{u}}_2(t) = 2^{-1/2}(1, 1)^{\mathrm{T}}.$$

However, computing the "smooth" eigenvectors, such as $\widetilde{\mathbf{u}}_1(t)$, $\widetilde{\mathbf{u}}_2(t)$, may be prohibitively expensive at points where algebraic multiplicity of eigenvalues changes for realistic large scale eigenvalue problems, which depend on many parameters (t in our case). At the same time, the formulas $\widetilde{\lambda}_i'(t) = \mathbf{u}_i^{\mathrm{T}}(t)\mathbf{A}'(t)\mathbf{u}_i(t)$, $i = 1, 2$ do not hold any longer if an arbitrary eigenvector $\mathbf{u}_i(t)$ is used in place of the smooth one, $\widetilde{\mathbf{u}}_i(t)$, $i = 1, 2$. Indeed, as in Example 1 above, we put at $t = t_k$, $k = 0, \pm 1, \pm 2, \ldots$

$$\mathbf{u}_1(t_k) = (\sin(\phi), \cos(\phi))^{\mathrm{T}},$$
$$\mathbf{u}_2(t_k) = (\cos(\phi), -\sin(\phi))^{\mathrm{T}},$$

$\phi \in [0, 2\pi)$. Then, unless $\phi = 3\pi/4$ or $\phi = 7\pi/4$,

$$(-1)^{k+1} = \widetilde{\lambda}_1'(t_k) \neq \mathbf{u}_1^{\mathrm{T}}(t_k)\mathbf{A}'(t_k)\mathbf{u}_1(t_k) = (-1)^k \sin(2\phi),$$
$$(-1)^k = \widetilde{\lambda}_2'(t_k) \neq \mathbf{u}_2^{\mathrm{T}}(t_k)\mathbf{A}'(t_k)\mathbf{u}_2(t_k) = (-1)^{k+1} \sin(2\phi).$$

Thus formulas (1) *agree with* but *do not follow from* the well-known expressions for the derivatives of the individual eigenvalues of algebraic multiplicity one, particularly in higher-dimensional cases.

In this note we establish generalizations (1) for higher-dimensional cases, where in place of $\operatorname{tr}\mathbf{A}(t)$ and $\det\mathbf{A}(t)$ we have general symmetric polynomials of the eigenvalues. We conclude the introduction by noting that sensitivity analysis in the presence of multiple eigenvalues is a well known and well studied issue. For alternative approaches to the problem we refer to the two review papers [3,5] and references therein. The main advantage of the present approach is its exactness yet computational simplicity; indeed, it only requires computing the same information as one would need for the case without eigenvalue multiplicity, that is: eigenvalues, corresponding eigenvectors, and derivatives of the matrices with respect to the parameter. Of course this comes at the cost of only providing sensitivity information about the symmetric polynomials of the eigenvalues and not individual eigenvalues, which may not be sufficient for certain applications.

2 Sensitivity of symmetric polynomials of eigenvalues

To simplify the notation, we consider the case of real symmetric matrices $\mathbb{S}^m$, but all results hold true for complex self-adjoint matrices as well. For a pair of smooth matrix functions $\mathbf{K}, \mathbf{M} : \mathbb{R} \to \mathbb{S}^m$ such that $\mathbf{M}(t)$ is positive definite for every $t \in \mathbb{R}$ we consider a parametric generalized eigenvalue problem:

$$\mathbf{K}(t)\mathbf{v}(t) = \lambda(t)\mathbf{M}(t)\mathbf{v}(t). \tag{2}$$

We assume that (2) admits n eigenvalues isolated from the rest. That is, the eigenvalues satisfy

$$\cdots \leq \lambda_0(t) < \lambda_1(t) \leq \cdots \leq \lambda_n(t) < \lambda_{n+1}(t) \leq \cdots. \tag{3}$$

We let $E_i(t)$ denote the eigenspace corresponding to the eigenvalue $\lambda_i(t)$; that is, $E_i(t) = \{\mathbf{v} \in \mathbb{R}^m \mid \mathbf{K}(t)\mathbf{v} = \lambda_i(t)\mathbf{M}(t)\mathbf{v}\}$. We furthermore let $E(t) = E_1(t) + \cdots + E_n(t)$ be the joint eigenspace of the eigenvalues $\lambda_1(t), \ldots, \lambda_n(t)$. A crucial fact going back to Rellich 1953 is that this space depends smoothly on the parameter t, see [2]. In particular, there exists a basis $\mathbf{v}_1(t), \ldots, \mathbf{v}_n(t)$ for $E(t)$ that depends smoothly on t. We will prove that there is another basis for $E(t)$ satisfying certain additional requirements.

Lemma 1 *Let* $\mathbf{K},\mathbf{M}:\mathbb{R}\to\mathbb{S}^m$ *be a smooth family of symmetric matrices as described above with* n *generalized eigenvalues satisfying* (3)*. Assume furthermore that* $\mathbf{u}_1,\ldots,\mathbf{u}_n\in\mathbb{R}^m$ *is an* $\mathbf{M}(0)$*-orthonormal set of eigenvectors for* (2) *at* $t=0$ *corresponding to eigenvalues* $\lambda_1(0),\ldots,\lambda_n(0)$*. Then we can find another basis* $\mathbf{w}_1(t),\ldots,\mathbf{w}_n(t)\in\mathbb{R}^m$ *for* $E(t)$ *such that, for all* $k,\ell=1,\ldots,n$, $t\in\mathbb{R}$*:*

1. $\mathbf{w}_k(t)$ *is a smooth function of* t*;*
2. $\mathbf{w}_k(t)$ *and* $\mathbf{w}_\ell(t)$ *are* $\mathbf{M}(t)$*-orthogonal, that is,* $\mathbf{w}_k^{\mathrm{T}}(t)\mathbf{M}(t)\mathbf{w}_\ell(t)=\delta_{k\ell}$*, where* $\delta_{k\ell}$ *is Kronecker's delta;*
3. $\mathbf{w}_k(0)=\mathbf{u}_k$*.*

Proof Applying Gram–Schmidt orthogonalization process to the basis $\mathbf{v}_k(t)$, $k=1,\ldots,n$ we obtain a $\mathbf{M}(t)$-orthonormal basis for $E(t)$ smoothly depending on the parameter; we denote this basis again with $\mathbf{v}_k(t)$, $k=1,\ldots,n$. Let us write $(\mathbf{u}_1,\ldots,\mathbf{u}_n)$ in terms of the latter basis as $(\mathbf{v}_1(0),\ldots,\mathbf{v}_n(0))\mathbf{U}$, where $\mathbf{U}\in O(n)$ is a $n\times n$ orthogonal matrix. We now define our new basis as $(\mathbf{w}_1(t),\ldots,\mathbf{w}_n(t)):=(\mathbf{v}_1(t),\ldots,\mathbf{v}_n(t))\mathbf{U}$ and obtain a basis for $E(t)$ which satisfies conditions 1, 2, and 3. □

Theorem 1 *Let* $\mathbf{K},\mathbf{M}:\mathbb{R}\to\mathbb{S}^m$ *be a smooth family of symmetric matrices as described above with n generalized eigenvalues satisfying* (3)*. Then the symmetric polynomials*

$$s_k(t)=\sum_{1\le i_1<\cdots<i_k\le n}\lambda_{i_1}(t)\cdots\lambda_{i_k}(t), \tag{4}$$

$k=1,\ldots,n$ *are smooth functions and their derivatives at* $t=0$ *are given by*

$$s_k'(0)=\sum_{1\le i_1<\cdots i_k\le n}\sum_{\ell=1}^{k}\lambda_{i_1}(0)\cdots\lambda_{i_{\ell-1}}(0)\times \\ \times\mathbf{u}_{i_\ell}^{\mathrm{T}}[\mathbf{K}'(0)-\lambda_{i_\ell}(0)\mathbf{M}'(0)]\mathbf{u}_{i_\ell}\cdot\lambda_{i_{\ell+1}}(0)\cdots\lambda_{i_k}(0), \tag{5}$$

where $\mathbf{u}_1,\ldots,\mathbf{u}_n\in\mathbb{R}^m$ *is an* $\mathbf{M}(0)$*-orthonormal set of eigenvectors for* (2) *at* $t=0$ *corresponding to eigenvalues* $\lambda_1(0),\ldots,\lambda_n(0)$*.*

Proof Choose the basis $\mathbf{w}_1(t),\ldots,\mathbf{w}_n(t)$ for $E(t)$ secured by Lemma 1. We now define the matrix families $\hat{\mathbf{K}},\hat{\mathbf{M}}:\mathbb{R}\to\mathbb{S}^n$ with elements

$$\hat{k}_{k\ell}(t)=\mathbf{w}_k^{\mathrm{T}}(t)\mathbf{K}(t)\mathbf{w}_\ell(t),$$
$$\hat{m}_{k\ell}(t)=\mathbf{w}_k^{\mathrm{T}}(t)\mathbf{M}(t)\mathbf{w}_\ell(t),$$

$k,\ell=1,\ldots,n$. That is, $\hat{\mathbf{K}}(t)$, $\hat{\mathbf{M}}(t)$ are restrictions of $\mathbf{K}(t)$, $\mathbf{M}(t)$ to $E(t)$ expressed in the basis $\mathbf{w}_k(t)$, $k=1,\ldots,n$. As this is an $\mathbf{M}(t)$-orthonormal basis we have that $\hat{\mathbf{M}}(t)\equiv\mathbf{I}$ or equivalently that $\hat{m}_{k\ell}(t)=\delta_{k\ell}$, $k,\ell=1,\ldots,n$. It is easy to verify that the eigenvalue problem $\hat{\mathbf{K}}(t)\mathbf{v}=\lambda(t)\hat{\mathbf{M}}(t)\mathbf{v}=\lambda(t)\mathbf{v}$ shares its n eigenvalues with the problem (2), namely $\lambda_1(t),\ldots,\lambda_n(t)$.

Let us now consider the characteristic polynomial $p_t(\lambda)=\det[\hat{\mathbf{K}}(t)-\lambda\mathbf{I}]$. The matrix $\hat{\mathbf{K}}(t)-\lambda\mathbf{I}$ has components $\hat{k}_{k\ell}(t)-\lambda\delta_{k\ell}$ and the characteristic polynomial can be written as

$$p_t(\lambda)=\sum_{\text{permutations }\sigma}\operatorname{sgn}\sigma\prod_{k=1}^{n}[\hat{k}_{k,\sigma(k)}(t)-\lambda\delta_{k,\sigma(k)}].$$

Differentiating the product above with respect to t and evaluating the derivative at $t=0$ we get:

$$\frac{\mathrm{d}}{\mathrm{d}t}\prod_{k=1}^{n}[\hat{k}_{k,\sigma(k)}(t)-\lambda\delta_{k,\sigma(k)}]\bigg|_{t=0}= \\ \sum_{k=1}^{n}\left\{\hat{k}'_{k,\sigma(k)}(0)\cdot\prod_{\ell\ne k}[\hat{k}_{\ell,\sigma(\ell)}(0)-\lambda\delta_{\ell,\sigma(\ell)}]\right\}. \tag{6}$$

Since $\hat{\mathbf{K}}(0)=\operatorname{diag}[\lambda_1(0),\ldots,\lambda_n(0)]$ owing to condition 3 of Lemma 1, we immediately infer that the right hand side sum in (6) is zero unless σ is identity. As a result, we get the equality

$$\frac{\mathrm{d}}{\mathrm{d}t}p_t(\lambda)|_{t=0}=\sum_{k=1}^{n}\hat{k}'_{kk}(0)\cdot\prod_{\ell\ne k}[\lambda_\ell(0)-\lambda]. \tag{7}$$

Owing to the symmetry of $\mathbf{M}(t)$ we have

$$0=\hat{m}'_{kk}(0)=\mathbf{w}_k'(0)^T\mathbf{M}(0)\mathbf{w}_k(0)+\mathbf{w}_k(0)^T\mathbf{M}'(0)\mathbf{w}_k(0) \\ +\mathbf{w}_k(0)^T\mathbf{M}(0)\mathbf{w}_k'(0)=\mathbf{u}_k^T\mathbf{M}'(0)\mathbf{u}_k+2\mathbf{w}_k'(0)^T\mathbf{M}(0)\mathbf{u}_k.$$

Similarly, utilizing the fact that $\mathbf{u}_k$ is a generalized eigenvector corresponding to $\lambda_k(0)$ we get

$$\begin{aligned}\hat{k}'_{kk}(0)&=\mathbf{u}_k^T\mathbf{K}'(0)\mathbf{u}_k+2\mathbf{w}_k'(0)^T\mathbf{K}(0)\mathbf{u}_k\\&=\mathbf{u}_k^T\mathbf{K}'(0)\mathbf{u}_k+2\lambda_k(0)\mathbf{w}_k'(0)^T\mathbf{M}(0)\mathbf{u}_k\\&=\mathbf{u}_k^T\mathbf{K}'(0)\mathbf{u}_k-\lambda_k(0)\mathbf{u}_k^T\mathbf{M}'(0)\mathbf{u}_k.\end{aligned} \tag{8}$$

Substituting (8) into (7) results in:

$$\frac{\mathrm{d}}{\mathrm{d}t}p_t(\lambda)|_{t=0}= \\ \sum_{k=1}^{n}\{\mathbf{u}_k^{\mathrm{T}}[\mathbf{K}'(0)-\lambda_k(0)\mathbf{M}'(0)]\mathbf{u}_k\cdot\prod_{\ell\ne k}[\lambda_\ell(0)-\lambda]\}. \tag{9}$$

Let us denote by $a_k(t)$, $k=0,\ldots,n$, the coefficient of the characteristic polynomial in front of λ^{n-k}. They are related to the symmetric polynomials (4) as $s_k(t)=(-1)^{n-k}a_k(t)$, $k=1,\ldots,n$. As a result, $s_k(t)$, $k=1,\ldots,n$ are smooth functions of t. Finally, from (9) we obtain (5). □

Remark 2 Of course, there is nothing special about $t=0$ and, with obvious modifications, formulas (5) allow us to evaluate $s_k'(t)$, $k=1,\ldots,n$ for an arbitrary $t\in\mathbb{R}$.

3 Application to shape optimization

In this section we briefly describe a problem where we have successfully used the presented approach to multiple eigenvalues; the interested reader is referred to [4] for more details. The problem concerns finding a shape of a drum, or a vibrating membrane, where the first four frequencies of the spectrum are given. These frequencies should be in the proportion 2 : 3 : 3 : 4, and as a result the eigenvalues of the Laplace operator have to be in the proportion 4 : 9 : 9 : 16. Therefore, for the final shape we want $\lambda_2 = \lambda_3 = \frac{9}{4}\lambda_1$, and $\lambda_4 = 4\lambda_1$. These requirements on the eigenvalues are far from determining the shape of the drum, so we employ them as constraints and minimize the perimeter of the drum for regularization purposes. Numerically, we discretize the problem using the isogeometric analysis approach; the boundary is parametrized using B-splines with 40 control (design) variables.

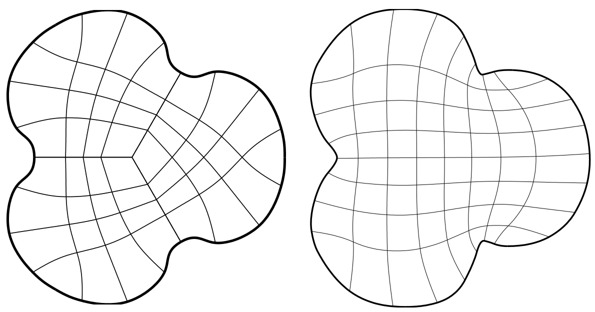

Fig. 1 Left: membrane shape found by imposing the exact 120° symmetry implying only smooth eigenvalues. Right: the result obtained without imposing symmetry; non-smooth eigenvalues are handled by the method described in this note.

When we impose the exact 120° symmetry on the family of admissible shapes, see Fig. 1, then the constraint $\lambda_2 = \lambda_3$ is automatically satisfied at all times and as a result all four eigenvalues become smooth functions of the parameters, defining the symmetric shape. However, without explicitly imposing the exact symmetry the desired double eigenvalue $\lambda_2 = \lambda_3$ causes problems for the optimization. Each time λ_2 and λ_3 "cross" during the optimization process, the employed non-linear programming algorithm finds itself at a non-differentiable point in the space of parameters, defining the shape. As a result, the non-linear algorithm gets "thrown off" and in fact we never obtained convergence in this setting, see Fig. 2. However, when we replace the non-smooth constraints $\lambda_2 = \mu$ and $\lambda_3 = \mu$ with the equivalent smooth constraints $\lambda_2 + \lambda_3 = 2\mu$ and $\lambda_2\lambda_3 = \mu^2$ with derivatives evaluated on the basis of (5), the optimization algorithm succeeds, see the right hand side of Fig. 1 and Fig. 3.

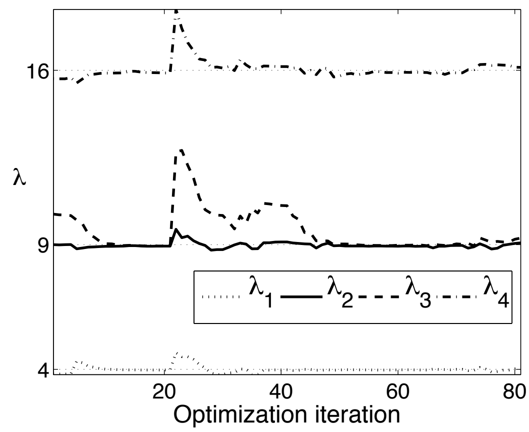

Fig. 2 Behaviour of (normalized) eigenvalues as functions of the optimization iteration: ignoring the non-smoothness of the eigenvalues results in large "jumps" at non-smooth points when λ_2 and λ_3 cross. In the end, optimization fails to converge to a desired precision.

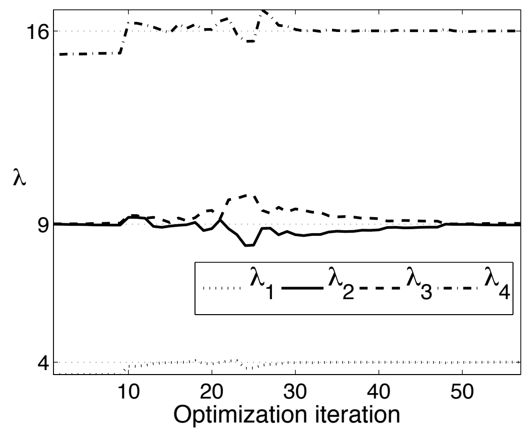

Fig. 3 Behaviour of (normalized) eigenvalues as functions of the optimization iteration: replacing the non-smooth double-eigenvalue constraints with their smooth equivalents based on evaluating symmetric polynomials allows us to successfully compute the desired shape.

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