

# Differentiating Generalized Eigen and Singular Value Decompositions

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The derivatives of eigenvalues and eigenvectors (and singular values and vectors) are used in many places in multivariate data analysis. This paper reviews formulas for these derivatives and discusses several applications. R code implementing the basic formulas and applications is included. The results extend, generalize, correct, and improve the results of De Leeuw ([2007](#)).

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**Note:** This is a working manuscript which will be expanded/updated frequently. All suggestions for improvement are welcome. All qmd, tex, html, pdf, R, and C files are in the public domain. Attribution will be appreciated, but is not required. Files can be found at <https://github.com/deleeuw/generalized-eigen-derivatives>

# 1 Introduction

Suppose  $A$  and  $B$  are real symmetric matrices of order  $n$ , with  $B$  positive definite (PSD, from now on). Generalized eigenvalues and eigenvectors are defined as the solutions  $(x, \lambda)$  of the system of equations

$$Ax = \lambda Bx, \quad (1a)$$

$$x' Bx = 1. \quad (1b)$$

We call this a GEV system, short for generalized eigenvalue system.

The properties of the solutions of the system (1a),(1b) can be found in any textbook on matrix algebra, for example in my personal favorite Wilkinson (1965). We briefly summarise them here.

Solving equation (1a) is equivalent to solving the determinantal equation  $\det(A - \lambda B) = 0$ . The polynomial  $\det(A - \lambda B)$  is of degree  $n$ , and consequently has  $n$  roots. Because  $A$  is symmetric and  $B$  is positive definite all  $n$  roots are real. Note that  $A$  can be indefinite and/or singular, which means that some roots can be negative or zero.

If  $\lambda_s \neq \lambda_t$  are two solutions of the determinantal equation then the corresponding eigenvectors, which are defined up to a scale factor,  $x_s$  and  $x_t$  are B-orthogonal, i.e.  $x_s' Bx_t = 0$ . If  $\lambda_s$  is a root of multiplicity  $p$  then there are  $p$  corresponding eigenvectors, spanning a  $p$ -dimensional subspace of  $\mathbb{R}^n$ , and these  $p$  eigenvectors can be chosen to be B-orthogonal as well. If we use the normalization in (1b) it follows that there exists a non-singular matrix  $X$  and a diagonal  $\Lambda$  such that  $X' B X = I$  and  $A X = B X \Lambda$ , which implies  $X' A X = \Lambda$ . If all roots are different the solution  $(X, \Lambda)$  is unique up to a permutation of the columns of  $X$ , and we can eliminate this non-uniqueness by requiring that  $\lambda_1 > \lambda_2 > \dots > \lambda_n$ . If there are multiple roots, and we require  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ , the solution is unique up to a rotation within each of the subspaces associated with multiple roots.

If  $\lambda_s$  is a simple eigenvalue, i.e. it is different from all other roots, then both  $\lambda_s$  and  $x_s$  are differentiable at  $(A, B)$  (see Wilkinson (1965), chapter 2, and for much more detail Kato (1976)). Suppose the matrices  $\Delta_A$  and  $\Delta_B$  are real and symmetric perturbations. Define<sup>12</sup>

$$A(\epsilon) := A + \epsilon \Delta_A + o(\epsilon), \quad (2a)$$

$$B(\epsilon) := B + \epsilon \Delta_B + o(\epsilon). \quad (2b)$$

Differentiability of  $\lambda_s$  and  $x_s$  implies that the differentials

$$d\lambda_s := \lim_{\epsilon \rightarrow 0} \frac{\lambda_s(A(\epsilon), B(\epsilon)) - \lambda_s(A, B)}{\epsilon}, \quad (3a)$$

<sup>1</sup>Here  $o(\epsilon)$  is any function of  $\epsilon$  satisfying  $\lim_{\epsilon \rightarrow 0} o(\epsilon)/\epsilon = 0$ .

<sup>2</sup>The symbol  $:=$  is used for definitions.

and

$$dx_s := \lim_{\epsilon \rightarrow 0} \frac{x_s(A(\epsilon), B(\epsilon)) - x_s(A, B)}{\epsilon} \quad (3b)$$

exist. Our notation suppresses the dependence of  $d\lambda_s$  and  $dx_s$  on  $(A, B)$  and on  $(\Delta_A, \Delta_B)$  because for our purposes these are just fixed constants.

## 2 Perturbation

### 2.1 Basic Perturbations

We study the effect of symmetric perturbations  $A + \epsilon \Delta_A + o(\epsilon)$  and  $B + \epsilon \Delta_B + o(\epsilon)$  of  $A$  and  $B$  on the eigenvalues  $\lambda_s$  and their corresponding eigenvectors  $x_s$ . Throughout we assume that  $\lambda_s$  has multiplicity one, i.e. that  $\lambda_t \neq \lambda_s$  if  $t \neq s$ . Note that this does not mean all eigenvalues need to be different. Also note that if  $\epsilon$  is small enough then  $B(\epsilon)$  is still positive definite and  $\lambda_s(A(\epsilon), B(\epsilon))$  is still a simple eigenvalue.

To find  $d\lambda_s$  and  $dx_s$  we must solve the equations

$$(A + \epsilon \Delta_A + o(\epsilon))(x_s + \epsilon dx_s + o(\epsilon)) = (B + \epsilon \Delta_B + o(\epsilon))(x_s + \epsilon dx_s + o(\epsilon))(\lambda_s + \epsilon d\lambda_s + o(\epsilon)), \quad (4a)$$

and

$$(x_s + \epsilon dx_s + o(\epsilon))'(B + \epsilon \Delta_B + o(\epsilon))(x_s + \epsilon dx_s + o(\epsilon)) = 1. \quad (4b)$$

Expand (4a) and (4b) and only keep the first order terms. This gives

$$A dx_s + \Delta_A x_s = d\lambda_s B x_s + \lambda_s B dx_s + \lambda_s \Delta_B x_s, \quad (5a)$$

$$x_s' \Delta_B x_s + 2x_s' B dx_s = 0. \quad (5b)$$

Premultiply equation (5a) with  $x_s'$ . This gives

$$d\lambda_s = x_s'(\Delta_A - \lambda_s \Delta_B)x_s, \quad (6)$$

We next solve for  $dx_s$ . Write  $dx_s = X\alpha$ , where  $X$  is any complete set of eigenvectors from  $AX = BX\Lambda$ , normalized by  $X'BX = I$ . Then (5a) becomes

$$BX(\Lambda - \lambda_s I)\alpha = d\lambda_s Bx_s - (\Delta_A x_s - \lambda_s \Delta_B)x_s. \quad (7)$$

Premultiplying by  $X'$  gives

$$(\Lambda - \lambda_s I)\alpha = (d\lambda_s)e_s - X'(\Delta_A - \lambda_s \Delta_B)x_s, \quad (8)$$

with  $e_s$  a unit vector.<sup>3</sup> Both sides of (8) are vectors of length  $n$ . Using (6) we see that element  $s$  of both vectors is equal to zero. For  $t \neq s$  we obtain

$$\alpha_t = -\frac{x_t'(\Delta_A - \lambda_s \Delta_B)x_s}{\lambda_t - \lambda_s}, \quad (9)$$

---

<sup>3</sup>A unit vector  $e_s$  has element  $s$  equal to one and all other elements equal to zero.

and, using (5b),

$$\alpha_s = -\frac{1}{2}x'_s \Delta_B x_s. \quad (10)$$

Thus

$$dx_s = -\sum_{t \neq s} \frac{x'_t (\Delta_A - \lambda_s \Delta_B) x_s}{\lambda_t - \lambda_s} x_t - \frac{1}{2} (x'_s \Delta_B x_s) x_s. \quad (11)$$

The two equations (6) and (11) are the basic tools we use in this paper.

Equations (6) and (11) simplify in some important special cases. For example, we can perturb  $A$  but not  $B$ . Thus  $\Delta_B = 0$ , and

$$d\lambda_s = x'_s \Delta_A x_s, \quad (12a)$$

and

$$dx_s = -\sum_{t \neq s} \frac{x'_t \Delta_A x_s}{\lambda_t - \lambda_s} x_t. \quad (12b)$$

If, in addition,  $B = I$  we have perturbation equations for an SEV or simple eigenvalue problem. The case in which we perturb  $B$  and not  $A$  is handled in the same way. Other special cases and simplifications will be treated next.

## 2.2 Parametric Perturbations

If  $A$  and  $B$  are differentiable functions of a vector of  $q$  parameters  $\theta$  then

$$A(\theta + \epsilon d\theta) = A(\theta) + \epsilon \sum_{r=1}^q d\theta_r \mathcal{D}_r A + o(\epsilon), \quad (13a)$$

$$B(\theta + \epsilon d\theta) = B(\theta) + \epsilon \sum_{r=1}^q d\theta_r \mathcal{D}_r B + o(\epsilon). \quad (13b)$$

Here the  $\mathcal{D}_r A$  is a matrix with partial derivatives of  $A$  with respect to  $\theta_r$ , evaluated at  $\theta$ , and  $d\theta_r$  is element  $r$  of the perturbation  $d\theta$ . And similarly for  $B$ .

We now can apply equations (6) and (11) with

$$\Delta_A = \sum_{r=1}^q d\theta_r \mathcal{D}_r A, \quad (14a)$$

$$\Delta_B = \sum_{r=1}^q d\theta_r \mathcal{D}_r B. \quad (14b)$$

If  $A$  and  $B$  depend on two different sets of parameters then we can use the same equations with some of the  $\mathcal{D}_r A$  and some of the  $\mathcal{D}_r B$  equal to zero.

### 2.2.1 Linear Perturbations

In an important special case  $A$  and  $B$  are linear in  $\theta$ . So

$$A(\theta) = \sum_{r=1}^q \theta_r A_r, \quad (15a)$$

$$B(\theta) = \sum_{r=1}^q \theta_r B_r. \quad (15b)$$

In that case  $\Delta_A = \mathcal{D}_r A = A_r$  and  $\Delta_B = \mathcal{D}_r B = B_r$ .

### 2.2.2 Elementwise Perturbations

In an important special case of the linear case the parameters are all the  $n(n+1)$  elements of  $A$  and  $B$  on and above the diagonal. We have

$$A = \sum_{1 \leq i < j \leq n} a_{ij} E_{ij} + \sum_{i=1}^n a_{ii} E_i, \quad (16a)$$

$$B = \sum_{1 \leq i < j \leq n} b_{ij} E_{ij} + \sum_{i=1}^n b_{ii} E_i, \quad (16b)$$

with  $E_{ij} := e_i e_j' + e_j e_i'$  and  $E_i := e_i e_i'$ .

## 2.3 Perturbation Code

The code in Section 7 has the function `perturbGeigen()`, written in R (R Core Team (2024)), which has arguments  $a, b, da, db$  and  $p$ . The first four arguments are the values of  $A, B, \Delta_A, \Delta_B$ . The remaining argument  $p$  is a subset of  $\{1, 2, \dots, n\}$ , with  $1 \leq m \leq n$  elements. The program computes  $d\lambda_s$  and  $dx_s$  for all  $s \in p$  and returns them, respectively, in a vector with  $m$  elements and an  $n \times m$  matrix. The computations use (12a) and (12b).

The code section also has the function `perturbCheck()`, with the same arguments as `perturbGeigen()`, plus the additional argument  $eps$ , the value of  $\epsilon$ . The function computes generalized eigenvalues and eigenvectors of the pair  $(A + \epsilon \Delta_A, B + \epsilon \Delta_B)$  and compares them with the output of `perturbGeigen()`.

Our example uses two matrices  $A$  and  $B$  of order three. They are



|      | [,1]      | [,2]      | [,3]      |
|------|-----------|-----------|-----------|
| [1,] | +4.000000 | +1.000000 | +2.000000 |
| [2,] | +1.000000 | +5.000000 | +3.000000 |
| [3,] | +2.000000 | +3.000000 | +6.000000 |

|      | [,1]      | [,2]      | [,3]      |
|------|-----------|-----------|-----------|
| [1,] | +3.000000 | -1.000000 | -1.000000 |
| [2,] | -1.000000 | +3.000000 | -1.000000 |
| [3,] | -1.000000 | -1.000000 | +3.000000 |

The generalized eigen decomposition of  $A$  and  $B$  has eigenvalues

[1] +9.080056 +0.859087 +0.560857

and eigenvectors

|      | [,1]      | [,2]      | [,3]      |
|------|-----------|-----------|-----------|
| [1,] | +0.539749 | -0.410185 | -0.201044 |
| [2,] | +0.575284 | +0.290249 | -0.291211 |
| [3,] | +0.608749 | +0.015385 | +0.359428 |

The perturbations  $\Delta_A$  and  $\Delta_B$  we use are

|      | [,1]      | [,2]      | [,3]      |
|------|-----------|-----------|-----------|
| [1,] | +1.000000 | +0.000000 | +0.000000 |
| [2,] | +0.000000 | +0.000000 | +0.000000 |
| [3,] | +0.000000 | +0.000000 | +0.000000 |

|      | [,1]      | [,2]      | [,3]      |
|------|-----------|-----------|-----------|
| [1,] | +0.000000 | +0.000000 | +0.000000 |
| [2,] | +0.000000 | +0.000000 | +0.000000 |
| [3,] | +0.000000 | +0.000000 | +0.000000 |

So  $B$  is not perturbed at all. The output of `perturbEigen()` is

\$dl

```
[1] 0.29132948 0.16825178 0.04041874
```

\$dx

```
      [,1]      [,2]      [,3]
[1,] 0.013607411 -0.04105592 0.120297564
[2,] -0.004107324 -0.06503134 -0.072930515
[3,] -0.004992561 0.11578144 0.003499643
```

We run `perturbCheck()` with  $\epsilon$  equal to 0.01. The generalized eigenvalues and eigenvectors of  $A + \epsilon\Delta_A$  and  $B + \epsilon\Delta_B$  are

```
[1] +9.0829695442 +0.8607716139 +0.5612588419
```

```
      [,1]      [,2]      [,3]
[1,] +0.5398854997 -0.4105912934 -0.1998460332
[2,] +0.5752433377 +0.2896010798 -0.2919354673
[3,] +0.6086986633 +0.0165387642 +0.3594612728
```

and the first order approximations  $\Lambda + \epsilon d\Lambda$  and  $X + \epsilon dX$  are

```
[1] +9.0829688098 +0.8607699411 +0.5612612491
```

```
      [,1]      [,2]      [,3]
[1,] +0.5398855373 -0.4105956100 -0.1998411515
[2,] +0.5752433585 +0.2895982756 -0.2919398461
[3,] +0.6086986857 +0.0165432294 +0.3594628991
```

The approximation is very good, although this is not surprising given the small example and the separation of the eigenvalues. It does indicate our formula are probably OK.

## 3 Partial Derivatives

### 3.1 Basic Partial Derivatives

The parametric perturbation results can be easily translated into the language and notation for partial derivatives. Let's introduce the notation first. If  $f$  is a function of a vector  $\theta$  then the partial derivative with respect to  $\theta_r$  is  $\mathcal{D}_r f$ , defined by

$$\mathcal{D}_r f(\theta) := \lim_{\epsilon \rightarrow 0} \frac{f(\theta + \epsilon e_r) - f(\theta)}{\epsilon},$$

with  $e_r$  a unit vector.

To find partial derivatives we set  $d\theta = e_r$ . In our perturbation equations (14a) and (14b). Thus we only perturb  $\theta_r$ . We then have  $\Delta_A = \mathcal{D}_r A$  and  $\Delta_B = \mathcal{D}_r B$ , and thus

$$\mathcal{D}_r \lambda_s = x'_s (\mathcal{D}_r A - \lambda_s \mathcal{D}_r B) x_s, \quad (17a)$$

and

$$\mathcal{D}_r x_s = - \sum_{t \neq s} \frac{x'_t (\mathcal{D}_r A - \lambda_s \mathcal{D}_r B) x_s}{\lambda_t - \lambda_s} x_t - \frac{1}{2} (x'_s \mathcal{D}_r B x_s) x_s. \quad (17b)$$

For linear parametric perturbations we have the same equations for the partial derivatives with  $\mathcal{D}_r A = A_r$  and  $\mathcal{D}_r B = B_r$ .

### 3.2 Elementwise Perturbations

For elementwise perturbations there are some useful simplifications. If we apply (16a) and (16b) to (17a) and (17b) we get

$$\mathcal{D}_{ij}^A \lambda_s = \begin{cases} 2x_{is}x_{js} & \text{if } i \neq j, \\ x_{is}^2 & \text{if } i = j. \end{cases} \quad (18a)$$

$$\mathcal{D}_{ij}^B \lambda_s = \begin{cases} -2\lambda_s x_{is}x_{js} & \text{if } i \neq j, \\ -\lambda_s x_{is}^2 & \text{if } i = j. \end{cases} \quad (18b)$$

$$\mathcal{D}_{ij}^A x_s = \begin{cases} - \sum_{t \neq s} \frac{x_{is}x_{jt} + x_{js}x_{it}}{\lambda_t - \lambda_s} x_t & \text{if } i \neq j, \\ - \sum_{t \neq s} \frac{x_{is}x_{it}}{\lambda_t - \lambda_s} x_t & \text{if } i = j. \end{cases} \quad (18c)$$

$$\mathcal{D}_{ij}^B x_s = \begin{cases} \lambda_s \sum_{t \neq s} \frac{x_{is}x_{jt} + x_{js}x_{it}}{\lambda_t - \lambda_s} x_t - x_{is}x_{js}x_s & \text{if } i \neq j, \\ \lambda_s \sum_{t \neq s} \frac{x_{is}x_{it}}{\lambda_t - \lambda_s} x_t - \frac{1}{2} x_{is}^2 x_s & \text{if } i = j. \end{cases} \quad (18d)$$

In (18a)-(18d) we use the somewhat ad-hoc notation  $\mathcal{D}_{ij}^A$  and  $\mathcal{D}_{ij}^B$  for the partial derivatives with respect to  $a_{ij}$  and  $b_{ij}$ .

As an aside, instead of deriving (18a)-(18d) from (17a) and (17b) we could also have used the chain rule to derive (17a) and (17b) from (18a)-(18d). This looks like

$$\mathcal{D}_r \lambda_s = \sum_{1 \leq i \leq j \leq n} \sum \mathcal{D}_{ij}^A \lambda_s \mathcal{D}_r a_{ij} + \sum_{1 \leq i \leq j \leq n} \sum \mathcal{D}_{ij}^B \lambda_s \mathcal{D}_r b_{ij}, \quad (19a)$$

$$\mathcal{D}_r x_s = \sum_{1 \leq i \leq j \leq n} \sum \mathcal{D}_{ij}^A x_s \mathcal{D}_r a_{ij} + \sum_{1 \leq i \leq j \leq n} \sum \mathcal{D}_{ij}^B x_s \mathcal{D}_r b_{ij}. \quad (19b)$$

### 3.3 Second Order Partial

For various purposes in data analysis, such as Newton's method or asymptotic bias correction, we need the second derivatives of the eigenvalues and eigenvectors.

We start by differentiating equation (17a) with respect to  $\theta_u$ . Define the abbreviations  $C_{rs} := \mathcal{D}_r A - \lambda_s \mathcal{D}_r B$  and  $C_{rus} := \mathcal{D}_{ru} A - \lambda_s \mathcal{D}_{ru} B$ . This gives

$$\mathcal{D}_{ur} \lambda_s = 2(d_u x_s)' C_{rs} x_s + x_s' C_{rus} x_s - (d_u \lambda_s) x_s' \mathcal{D}_r B x_s, \quad (20)$$

We could expand this further by substituting  $d_u \lambda_s$  and  $d_u x_s$  from (17a) and (17b). But in computation we will use (20) as is, even though (20) does not show immediately that for each  $s$  the Hessian  $\mathcal{D}_{ru} \lambda_s$  is a symmetric matrix of order  $q$ . Note that in the linear case  $\mathcal{D}_{ru} A = \mathcal{D}_{ru} B = 0$ , so the middle term on the right disappears.

The logical next step is to differentiate (17b) with respect to  $\theta_u$ . We compute the second partials for one single element  $x_{ks}$  of  $X$  at a time. For each element  $x_{ks}$  the Hessian will be a symmetric matrix of order  $q$ . From (17b)

$$\mathcal{D}_r x_{ks} = - \sum_{t \neq s} \frac{x_t' C_{rs} x_s}{\lambda_t - \lambda_s} x_{kt} - \frac{1}{2} (x_s' \mathcal{D}_r B x_s) x_{ks}. \quad (21)$$

We start by working on the first term on the right of (21). Differentiating with respect to  $\theta_u$  gives

$$\mathcal{D}_u \left\{ \frac{x_t' C_{rs} x_s}{\lambda_t - \lambda_s} x_{kt} \right\} = \frac{x_t' C_{rs} x_s}{\lambda_t - \lambda_s} d_u x_{kt} + \mathcal{D}_u \left\{ \frac{x_t' C_{rs} x_s}{\lambda_t - \lambda_s} \right\} x_{kt}. \quad (22)$$

The derivative in the second term on the right of (22) evaluates to

$$\mathcal{D}_u \left\{ \frac{x_t' C_{rs} x_s}{\lambda_t - \lambda_s} \right\} = \frac{(\lambda_t - \lambda_s) \mathcal{D}_u \{x_t' C_{rs} x_s\} - x_t' C_{rs} x_s (d_u \lambda_t - d_u \lambda_s)}{(\lambda_t - \lambda_s)^2}. \quad (23)$$

The derivative in the first term of the numerator on the right of (23) is

$$\mathcal{D}_u \{x'_t C_{rs} x_s\} = (d_u x_t)' C_{rs} x_s + x'_t C_{rs} d_u x_s + x'_t C_{rus} x_s - (d_u \lambda_s) x'_t (\mathcal{D}_r B) x_s. \quad (24)$$

And finally, differentiating the last term in (21),

$$\mathcal{D}_u \{(x'_s \mathcal{D}_r B x_s) x_{ks}\} = \{2(d_u x_s)' \mathcal{D}_r B x_s + x'_s \mathcal{D}_{ru} B x_s\} x_{ks} + (x'_s \mathcal{D}_r B x_s) d_u x_{ks}. \quad (25)$$

We combine the results in (22)-(25) into one big equation. The resulting formula is pretty horrendous, but think of it as a recipe for calculation, not as a beautiful object in its own right.

$$\begin{aligned} \mathcal{D}_{ru} x_{ks} = & - \sum_{t \neq s}^n \left\{ \frac{x'_t C_{rs} x_s}{\lambda_t - \lambda_s} d_u x_{kt} + \right. \\ & + \frac{(d_u x_t)' C_{rs} x_s + x'_t C_{rs} (d_u x_s) + x'_t C_{rus} x_s - (d_u \lambda_s) x'_t (\mathcal{D}_r B) x_s}{\lambda_t - \lambda_s} x_{kt} + \\ & \left. - \frac{x'_t C_{rs} x_s (d_u \lambda_t - d_u \lambda_s)}{(\lambda_t - \lambda_s)^2} x_{kt} \right\} + \\ & - \{(d_u x_s)' \mathcal{D}_r B x_s + x'_s \mathcal{D}_{ru} B x_s\} x_{ks} - \frac{1}{2} (x'_s \mathcal{D}_r B x_s) d_u x_{ks}. \end{aligned} \quad (26)$$

There are simplifications in the linear case, where the second derivatives of  $A$  and  $B$  are zero, and we can replace  $\mathcal{D}_r A$  and  $\mathcal{D}_r B$  in (26) by  $A_r$  and  $B_r$ . Thus  $C_{rs} = A_r - \lambda_s B_r$ . Also  $C_{rus} = 0$  and  $\mathcal{D}_{ru} B = 0$ . Thus equations (20) and (26) become

$$\mathcal{D}_{ru} \lambda_s = 2(d_u x_s)' C_{rs} x_s - d_u \lambda_s x'_s B_r x_s, \quad (27)$$

and

$$\begin{aligned} \mathcal{D}_{ru} x_{ks} = & - \sum_{t \neq s} \left\{ \frac{x'_t C_{rs} x_s}{\lambda_t - \lambda_s} d_u x_{kt} \right. \\ & + \frac{(d_u x_t)' C_{rs} x_s + x'_t C_{rs} d_u x_s - (d_u \lambda_s) x'_t B_r x_s}{\lambda_t - \lambda_s} x_{kt} \\ & \left. - \frac{x'_t C_{rs} x_s (d_u \lambda_t - d_u \lambda_s)}{(\lambda_t - \lambda_s)^2} x_{kt} \right\} \\ & - ((d_u x_s)' B_r x_s) x_{ks} - \frac{1}{2} (x'_s B_r x_s) d_u x_{ks}. \end{aligned} \quad (28)$$

There are more simplifications for SEV problems where  $B$  does not depend on  $\theta$  and thus  $\mathcal{D}B = 0$ .

### 3.4 Partial Derivative Code

The functions `partialGeigen()` and `partialCheck()` can be used for linear perturbations. They have both have arguments  $\theta$ ,  $a$ ,  $b$ ,  $s$ , where  $a$  and  $b$  are lists of matrices of lengths  $q$  and  $p$  and  $\theta$  is a vector of length  $p + q$ . The last  $q$  matrices in the list  $a$  are zero, as are the first  $p$  matrices in the list  $b$ . The index  $1 \leq s \leq n$  dictates which eigen-pair we study.

`partialGeigen()` uses the formulas (17a) and (17b), while `partialCheck` computes numerical derivatives using `grad()` and `jacobian()` from the `numDeriv` package (Gilbert and Varadhan (2019)). For our example we use the same  $A$  and  $B$  as before, and we use elementwise perturbation. For the dominant eigenvalue `partialGeigen()` gives the derivatives with respect to the elements of  $A$  and  $B$  as

We also used `partialCheck()` to compute numerical derivatives. The maximum absolute difference between the numerical and analytical partials of the eigenvalue is

The `partialGeigen()` function also gives the partials of the dominant eigenvector. The partials of the three eigenvector elements with respect to the elements of  $A$  are

and those with respect to  $B$  are

The maximum absolute differences between the numerical and analytical partials of the eigenvector are, for  $A$  and  $B$ ,

In elementwise perturbation `partialGeigen()` uses equations (17a) and (17b) and consequently needs lists of binary sparse matrices as arguments. This is very wasteful, both in memory and speed, given the fact that we also have the compact equations (18a) and (18). We have added the more specialized function `partialElement()` that uses these compact equations. It does not use  $\theta$  and the lists with the  $A_r$  and  $B_r$ . It gives the same results as `partialGeigen()`, but is much faster.

The function `hessianGeigenEval()` computes the second partials of the eigenvalues for linear perturbations. It has the same arguments as `partialGeigen()`. The function returns a list with the second partials of the eigenvalues.

`hessianCheckEval()` that computes numerical second partials. Even in our small example the Hessian is already of order 12, so we do not show the actual matrix. We do show that the maximum absolute difference between the numerical and analytical second partials of the eigenvalue is

## 4 Generalized SVD

Suppose  $F$  is an  $n \times m$  matrix,  $G$  is a positive definite matrix of order  $n$ , and  $H$  is a positive definite matrix of order  $m$ . We suppose without loss of generality that  $n \geq m$ . The generalized singular value problem for the triple  $(F, G, H)$  is to find solutions to the system

$$Fy = \lambda Gx, \quad (29a)$$

$$F'x = \lambda Hy, \quad (29b)$$

$$x'Gx + y'Hy = 1, \quad (29c)$$

We refer to this as a GSV system, short for generalized singular value system.

Now consider the GEV system

$$\begin{bmatrix} 0 & F \\ F' & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \lambda \begin{bmatrix} G & 0 \\ 0 & H \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}, \quad (30a)$$

with normalization

$$x'Gx + y'Hy = 1. \quad (30b)$$

It is easy to see that  $x$  and  $y$  satisfy (30a) and (30) if and only if they satisfy (29a) and (29b).

In GSV systems the normalization constraint (29c) is often replaced by the constraint  $x'Gx = y'Hy = 1$ . We now show that this does not change the solutions, except for multiplying the singular vectors with a scale factor  $\frac{1}{2}\sqrt{2}$ .

The GSV system has  $r = \text{rank}(F)$  solutions with  $\lambda_s > 0$ . For each of these solutions  $(\lambda_s, x_s, y_s)$  there is a mirror solution  $(-\lambda_s, x_s, -y_s)$ , and these  $2r$  solutions are also solutions of the GEV system. Because in GEV two solutions with different eigenvalues are orthogonal it follows that for a pair of mirror solutions with non-zero eigenvalue  $x'_s G x_s - y'_s H y_s = 0$ , and thus, using (30),  $x'_s G x_s = y'_s H y_s = \frac{1}{2}$ . In addition both systems have  $n + m - 2r$  solutions with zero eigenvalues, with eigenvectors in the direct sum of the null spaces of  $F$  and  $F'$ .

In summary, the solutions of the GEV and GSV systems for the ordered eigenvalues are

$$[\Lambda \quad 0 \quad 0 \quad -\Lambda], \quad (31a)$$

and for the corresponding eigenvectors

$$\begin{bmatrix} X & X_\perp & 0 & X \\ Y & 0 & Y_\perp & -Y \end{bmatrix}, \quad (31b)$$

with  $X_\perp$  a G-orthonormal basis for the null-space of  $F'$  and  $Y_\perp$  an H-orthonormal basis for the null-space of  $F$ . The four distinct parts of the solutions in (??) and (31) are of orders

$r, n - r, m - r$ , and  $r$ . We are only really interested in the first  $r$  solutions, for which the singular values can be chosen to be positive.

We now have enough information to apply our previous perturbation results to GSV systems, only considering perturbations of the form

$$\Delta_A = \begin{bmatrix} 0 & \Delta_F \\ \Delta'_F & 0 \end{bmatrix},$$

and

$$\Delta_B = \begin{bmatrix} \Delta_G & 0 \\ 0 & \Delta_H \end{bmatrix},$$

so that the perturbed system is still a GSV system.

From (6) we have

$$d\lambda_s = 2x'_s \Delta_F y_s - \lambda_s (x'_s \Delta_G x_s + y'_s \Delta_H y_s),$$

Now suppose  $s \leq r$ , so that  $\lambda_s$  is one of the first  $r$  positive singular values. From (11) we have

$$dx_s = - \sum_{\substack{t=1 \\ t \neq s}}^n \frac{x'_t (\Delta_A - \lambda_s \Delta_B) x_s}{\lambda_t - \lambda_s} x_t - \frac{1}{2} (x'_s \Delta_B x_s) x_s$$

Partial Derivatives

## 5 Applications

### 5.1 Principal Component Analysis

If we think of PCA as a function of the elements of covariance matrix then using our results is real simple. The elementwise perturbation results and partial derivative results from Section 3.2 apply directly, using  $B = I$  and  $\Delta_B = 0$ . If we interpret PCA as a function of the correlation matrix matters become slightly more complicated.  $A$  is still the covariance matrix, but  $B$  is now the diagonal of the covariance matrix. The  $\frac{1}{2}n(n+1)$  covariances are still the parameters, but the diagonal elements contribute to both  $A$  and  $B$ . Thus there are  $\frac{1}{2}n(n+1)$  design matrices  $A_r$  and  $B_r$ , where the  $B_r$  corresponding with off-diagonal elements are zero.

It is perhaps more interesting to interpret PCA as a function of the data matrix. Suppose we have  $m$  numerical variables, with variable  $j$  having  $k_j$  possible values. This defines  $q := \prod_{j=1}^m k_j$  possible profiles, which are vectors of length  $m$  with all combinations of the variable values. The data are the relative frequencies of these profiles, collected in a vector  $p$  of length  $q$ . Write  $G$  for the  $q \times m$  matrix of profiles.



The GEV problem for the principal component analysis (PCA) of a covariance matrix has

$$A = G'(P - pp')G, B = I$$

while for a PCA of the correlation matrix

$$A = G'(P - pp')G, B = \text{diag}(G'(P - pp')G)$$

From ...

$$\mathcal{D}_r A = g_r g_r' - (\mu e_r' + e_r \mu'),$$

with  $\mu := Gp$ .

From ...  $\mathcal{D}_r B = 0$ . From ...

$$\mathcal{D}_r B = \text{diag}(g_r g_r') - 2\mu_r$$

These can be used in (17b) and (17b).

$$\mathcal{D}_r \lambda_s = x_s' \{g_r g_r' - (\mu e_r' + e_r \mu') - \lambda_s \{\text{diag}(g_r g_r') - 2\mu_r\} x_s$$

Alternative data matrix  $Z$  and PCA is an SVD of  $JZ$ , which

Jackknife, Infinitesimal Jackknife

## 5.2 Canonical Analysis

In Canonical Analysis

$$A = \begin{bmatrix} 0 & F'G \\ G'F & 0 \end{bmatrix},$$

and

$$B = \begin{bmatrix} F'F & 0 \\ 0 & G'G \end{bmatrix}$$

Perturb  $F$  and  $G$ , which gives

$$\Delta_A = \begin{bmatrix} 0 & \Delta_F' G + F' \Delta_G \\ G' \Delta_F + F \Delta_G & 0 \end{bmatrix}$$

and

$$\Delta_B = \begin{bmatrix} \Delta_F' F + F' \Delta_F & 0 \\ 0 & \Delta_G' G + G' \Delta_G \end{bmatrix}$$

### 5.3 Multiple Correspondence Analysis

We could introduce Multiple Correspondence Analysis (MCA) as a form of canonical analysis and use the perturbation results from Section 5.2. Instead we go directly to a parametric approach.

Suppose we have  $m$  categorical variables, with variable  $j$  having  $k_j$  categories. This defines  $q := \prod_{j=1}^m k_j$  profiles, which are binary vectors of length  $\sum_{j=1}^m k_j$ . The data are the relative frequencies of the profiles (cf. Gifi (1990), chapter 2).

In

$$A = \sum_{r=1}^q p_r g_r g_r', B = \sum_{r=1}^q p_r G_r,$$

where  $p_r$  is the relative frequency of profile  $r$ , and  $g_r$  is the profile vector. Matri  $G_r$  is diagonal, with  $g_r$  on the diagonal.

This is a linear parametric model, and consequently we can apply the formulas from Section 2.2.1 to find the derivatives of the eigenvalues and eigenvectors with respect to the  $p_r$ .

$$\mathcal{D}_r \lambda_s = x_s' (g_r g_r' - \lambda_s \text{diag}(g_r g_r')) x_s, \quad (32a)$$

and

$$\mathcal{D}_r x_s = - \sum_{t \neq s} \frac{x_t' (A_r - \lambda_s B_r) x_s}{\lambda_t - \lambda_s} x_t - \frac{1}{2} (x_s' B_r x_s) x_s. \quad (32b)$$

### 5.4 Classical Multidimensional Scaling

In classical multidimensional scaling (MDS) we have a symmetric matrix  $D$  of squared dissimilarities.

$$\xi_{ij} = -\frac{1}{2} \left\{ \theta_{ij}^2 - \frac{1}{n} \sum_{l=1}^n \theta_{il}^2 - \frac{1}{n} \sum_{l=1}^n \theta_{lj}^2 + \frac{1}{n^2} \sum_{k=1}^n \sum_{l=1}^n \theta_{kl}^2 \right\}$$

$$A = \sum_{1 \leq i < j \leq n} \xi_{ij} E_{ij} + \sum_{i=1}^n \xi_{ii} E_i$$

## 5.5 Factor Analysis

## 5.6 Low rank Matrix Approximation

## 6 Discussion

If  $B$  is a singular, if  $B$  is indefinite. If  $A$  and  $B$  are not symmetric.

## 7 Code

## References

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