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## On Derivatives of Eigenvalues and Eigenvectors of the Generalized Eigenvalue Problem

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### 1 Differentiating eigenvalues and eigenvectors

There are two problems involved in differentiating eigenvalues and eigenvectors. The first is that the eigenvalues of a real matrix  $\mathbf{A}$  need not to be, in general, real numbers – they may be complex. The second problem is the possible occurrence of multiple eigenvalues. If the eigenvalues are complex, their corresponding eigenvectors are complex. However, for real symmetric matrices, their eigenvalues are real and hence their eigenvectors can be taken to be real as well. Let  $\mathbf{A}_0 \in \mathbb{R}^{n \times n}$  be a symmetric matrix and let  $\mathbf{v}_0$  be a normalized eigenvector associated with eigenvalue  $\lambda_0$  of  $\mathbf{A}_0$  so that the triplet  $(\mathbf{A}_0, \mathbf{v}_0, \lambda_0)$  satisfies the equation:

$$\mathbf{A}\mathbf{v} = \lambda\mathbf{v} \quad \text{and} \quad \mathbf{v}^\top \mathbf{v} = 1. \tag{1}$$

The  $n+1$  equations previously mentioned are implicit functions of the eigenvalues and eigenvectors of  $\mathbf{A}_0$ . To differentiate the eigenvalues and eigenvectors for  $\mathbf{A}_0$  we must show that there exists explicit functions  $\lambda = \lambda(\mathbf{A})$  and  $\mathbf{v} = \mathbf{v}(\mathbf{A})$  satisfying Equation (1) in a neighborhood of  $\mathbf{A}_0$ ,  $\mathcal{N}(\mathbf{A}_0) \subset \mathbb{R}^{n \times n}$

and that  $\lambda(\mathbf{A}_0) = \lambda_0$  and  $\mathbf{v}(\mathbf{A}_0) = \mathbf{v}_0$ . The second problem arises here. That is, the occurrence of multiple eigenvalues.

Consider that this is not the case and that all eigenvalues of  $\mathbf{A}_0$  are distinct and real. Then the implicit function theorem guarantees the existence of neighborhood  $\mathcal{N}(\mathbf{A}_0) \subset \mathbb{R}^{n \times n}$  where the function  $\lambda$  and  $\mathbf{v}$  exist and are  $C^\infty$  – i.e.  $\infty$  times differentiable – on  $\mathcal{N}(\mathbf{A}_0)$  and provided  $\lambda_0$  is a simple eigenvalue of  $\mathbf{A}_0$ . If, however, the  $\lambda_0$  is a multiple eigenvalue of  $\mathbf{A}_0$ , then the conditions of the implicit function theorem are not satisfied.

In general, and in machine learning, we deal with real symmetric matrices (covariance matrices, gram matrices, similarity matrices) so all their eigenvalues are real although their simplicity is not guaranteed. However, it is more the case that we deal with real symmetric and (at least) semi-positive and positive definite matrices, and hence all their eigenvalues are greater than or equal to zero. Again, simplicity of eigenvalues is not guaranteed.

## 1.1 The differentiable of eigenvalues and eigenvectors for the real symmetric case

Let  $\mathbf{A}_0 \in \mathbb{R}^{n \times n}$  be a symmetric matrix, and let  $\mathbf{v}_0$  be a normalized eigenvector of  $\mathbf{A}_0$  associated with an eigenvalue  $\lambda_0$  of  $\mathbf{A}_0$ . Then a real-valued function  $\lambda$  and a real vector function  $\mathbf{v}$  are defined for all  $\mathbf{A} \in \mathcal{N}(\mathbf{A}_0)$  where  $\mathcal{N}(\mathbf{A}_0) \subset \mathbb{R}^{n \times n}$  is a small neighborhood of  $\mathbf{A}_0$  and that:

$$\lambda(\mathbf{A}_0) = \lambda_0 \quad \mathbf{v}(\mathbf{A}_0) = \mathbf{v}_0 \quad \text{and} \quad (2)$$

$$\mathbf{A}\mathbf{v} = \lambda\mathbf{v} \quad \mathbf{v}^\top \mathbf{v} = 1 \quad \forall \mathbf{A} \in \mathcal{N}(\mathbf{A}_0). \quad (3)$$

Moreover, if the functions  $\lambda$  and  $\mathbf{v}$  are  $C^\infty$  in the neighborhood  $\mathcal{N}(\mathbf{A}_0)$ , then the derivative of eigenvalues and eigenvectors at  $\mathbf{A}_0$  are:

$$d\lambda = \mathbf{v}_0^\top (d\mathbf{A}) \mathbf{v}_0 \quad (4)$$

$$d\mathbf{v} = (\lambda_0 \mathbf{I} - \mathbf{A}_0)^+ (d\mathbf{A}) \mathbf{v}_0, \quad (5)$$

where  $(\lambda_0 \mathbf{I} - \mathbf{A}_0)^+$  is the generalized Moore–Penrose inverse of  $(\lambda_0 \mathbf{I} - \mathbf{A}_0)$ .

## 2 Derivatives of generalized eigenvalues and eigenvectors — *The symmetric case*

The generalized eigenvalue problem (GEP) for a pair of symmetric matrices  $\mathbf{A} \in \mathbb{R}^{n \times n}$  and  $\mathbf{B} \in \mathbb{R}^{n \times n}$  is defined by the system of equations:

$$\mathbf{A}\mathbf{v} = \lambda\mathbf{B}\mathbf{v} \quad \text{and} \quad \mathbf{v}^\top \mathbf{B}\mathbf{v} = 1. \quad (6)$$

Any solution  $(\mathbf{v}, \lambda)$  is a generalized eigen pair with  $\mathbf{v}$  the generalized eigenvector and  $\lambda$  the generalized eigenvalue.

Now suppose the matrices  $\mathbf{A}$  and  $\mathbf{B}$  are matrix valued functions of a parameter  $\theta$ . Then Equation (6) defines  $\mathbf{v}$  and  $\lambda$  implicitly as a function of  $\theta$ . Suppose  $\hat{\theta}$  is a point where  $\mathbf{B}$  is positive definite ( $\mathbf{B} \succ 0$ ), and that the eigenvalues  $\lambda$  are simple and positive. Also, consider that the matrix valued functions  $\mathbf{A}$  and  $\mathbf{B}$  are  $C^2$ , two times continuously differentiable, at  $\hat{\theta}$ . Then, the implicit function theorem guarantees that the eigenvalues and eigenvectors are differentiable at  $\hat{\theta}$  and the partial derivative of  $\lambda_j$  with respect to  $\theta$  is :

$$\frac{\partial \lambda_j}{\partial \theta} = \mathbf{v}_j^\top \left( \frac{\partial \mathbf{A}}{\partial \theta} - \lambda_j \frac{\partial \mathbf{B}}{\partial \theta} \right) \mathbf{v}_j, \quad 1 \leq j \leq n \quad (7)$$

If  $\mathbf{A}$  depends on one set of parameters and  $\mathbf{B}$  depends on another set of parameters, then this can be handled by concatenating the two sets of parameters and setting some of the partial derivatives to zero. To compute the derivative of eigenvectors with respect to  $\theta$ , let us define the matrix  $\mathbf{V}$  as the set of complete generalized eigenvectors, where  $\mathbf{V}$  is nonsingular, and rewrite the generalized eigenvalue problem (GEP) as follows :

$$\mathbf{A}\mathbf{V} = \mathbf{B}\mathbf{V}\mathbf{\Lambda} \quad \text{and} \quad \mathbf{V}^\top \mathbf{B}\mathbf{V} = \mathbf{I}, \quad (8)$$

where  $\mathbf{\Lambda} = \text{diag}(\lambda_1, \dots, \lambda_n)$ . Then the partial derivative of  $\mathbf{v}$  with respect to  $\theta$  is:

$$\frac{\partial \mathbf{v}_j}{\partial \theta} = -(\mathbf{A} - \lambda_j \mathbf{B})^- \left( \frac{\partial \mathbf{A}}{\partial \theta} - \lambda_j \frac{\partial \mathbf{B}}{\partial \theta} \right) \mathbf{v}_j - \frac{1}{2} \left( \mathbf{v}_j^\top \frac{\partial \mathbf{B}}{\partial \theta} \mathbf{v}_j \right) \mathbf{v}_j, \quad (9)$$

where  $1 \leq j \leq n$ , and  $(\mathbf{A} - \lambda \mathbf{B})^- = \mathbf{V}(\mathbf{\Lambda} - \lambda \mathbf{I})^+ \mathbf{V}^\top$ .

If  $\mathbf{B}$  does not depend on  $\theta$  then:

$$\frac{\partial \lambda}{\partial \theta} = \mathbf{v}^\top \frac{\partial \mathbf{A}}{\partial \theta} \mathbf{v} \quad (10)$$

$$\frac{\partial \mathbf{v}}{\partial \theta} = -(\mathbf{A} - \lambda \mathbf{B})^- \frac{\partial \mathbf{A}}{\partial \theta} \mathbf{v} \quad (11)$$

If in addition  $\mathbf{B} = \mathbf{I}$ , then

$$\frac{\partial \mathbf{v}}{\partial \theta} = -(\mathbf{A} - \lambda \mathbf{I})^+ \frac{\partial \mathbf{A}}{\partial \theta} \mathbf{v} \quad (12)$$

## References

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