

Making Covariance Matrices Positive Definite

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1 Introduction

When working on simulation projects involving animals and genetics, genetic parameters are obtained by searching the literature for estimates. There are seldom any studies that include all of the traits of interest in one comprehensive analysis. Instead, estimates are scavenged from several different sources. After putting these estimates together into one covariance matrix, the likelihood that the matrix is singular is greater than 0. When the matrix is singular, of course, it cannot be inverted and it cannot be used for simulating traits on animals. Thus, a method of forcing the matrix to be positive definite would be useful, as long as most of the correlations between traits are maintained close to the estimates that were found. Estimated parameters have non-zero standard errors, and thus, there is some flexibility in correlations that can be allowed.

Hayes and Hill (1981) presented the “bending” procedure to modify eigenvalues of singular matrices, and Jorjani et al.(2003) gave a weighted bending procedure. Finally, Meyer and Kirkpatrick (2010) presented bending using a penalized maximum likelihood method. To me, however, the bending procedure causes many correlations and actual variances to differ more than expected from the original values. For example, if the variance of one trait was 100, then after bending it could be 70. The variances at least should not differ very much before and after modification.

Thus, over the years I have played with different approaches, until I think I have one that works, at least to my satisfaction. So the objective

of this little paper is to present the method and share it with whomever wants to use it. There were some inconsistencies in the previous paper, and so they have been corrected in this version, hopefully. Also, the approach is a little different.

2 Example

To demonstrate the procedure, let

$$\mathbf{G} = \begin{pmatrix} 100 & 95 & 80 & 40 & 40 \\ 95 & 100 & 95 & 80 & 40 \\ 80 & 95 & 100 & 95 & 80 \\ 40 & 80 & 95 & 100 & 95 \\ 40 & 40 & 80 & 95 & 100 \end{pmatrix} = \mathbf{UDU}'.$$

The eigenvalues are the diagonals of \mathbf{D} ,

$$diag\mathbf{D} = (399.48 \quad 98.52 \quad 23.65 \quad -3.12 \quad -18.52).$$

2.1 Step 1

Sum together the negative eigenvalues and multiply by 2.

$$s = (-3.12 - 18.52) * 2 = -43.28.$$

Now square this value, multiply by 100 and add 1.

$$t = (s * s) * 100 + 1 = 187,316.84.$$

2.2 Step 2

Change the negative eigenvalues to positive by the following: Let n be a negative eigenvalue, and let p be the lowest positive eigenvalue. Then the new eigenvalue is

$$n^* = p \times (s - n) \times (s - n)/t.$$

For example, $n = -3.12$ becomes

$$n^* = 23.65 \times (-43.28 - n) \times (-43.28 - n) / 187316.84 = 0.20363,$$

and $n = -18.52$ becomes

$$n^* = 23.65 \times (-43.28 - n) \times (-43.28 - n) / 187316.84 = 0.07740.$$

2.3 Step 3

Reconstruct the covariance matrix using a modified \mathbf{D}

$$\mathbf{D}^* = \begin{pmatrix} 399.48 & 98.52 & 23.65 & 0.20363 & 0.07740 \end{pmatrix},$$

and

$$\mathbf{G}^* = \mathbf{U}\mathbf{D}^*\mathbf{U}'$$

$$\mathbf{G}^* = \begin{pmatrix} 103.18978 & 90.82704 & 79.43676 & 44.56754 & 37.06769 \\ 90.82704 & 106.54177 & 94.13679 & 74.06296 & 44.56754 \\ 79.43676 & 94.13679 & 102.46432 & 94.13679 & 79.43676 \\ 44.56754 & 74.06296 & 94.13679 & 106.54177 & 90.82704 \\ 37.06769 & 44.56754 & 79.43676 & 90.82704 & 103.18978 \end{pmatrix}.$$

3 Discussion

If \mathbf{G} and \mathbf{G}^* are converted to correlation matrices (\mathbf{C}), and then the differences between the two correlation matrices are calculated as

$$\mathbf{C}_{G^*} - \mathbf{C}_G = \begin{pmatrix} 0 & -0.084 & -0.027 & 0.025 & -0.041 \\ -0.084 & 0 & -0.049 & -0.105 & 0.025 \\ -0.027 & -0.049 & 0 & -0.049 & -0.027 \\ 0.025 & -0.105 & -0.049 & 0 & -0.084 \\ -0.041 & 0.025 & -0.027 & -0.084 & 0 \end{pmatrix}.$$

The changes are certainly within the standard errors of the original estimates. If the original estimates had much smaller standard errors, then this matrix would be less likely to have any negative eigenvalues.

The method described here does not have any known statistical properties or advantages, except that the resulting matrix is positive definite and relatively close to the input matrix. The “bending” procedure, on the other hand, also makes a matrix positive definite, and according to Hayes and Hill (1981) optimizes the selection indices that are constructed from the modified covariance matrix. I am not sure if this is a good property to have or not. I have not taken the time to repeat the Hayes and Hill (1981) study using the current method. I leave such a study to a clever and eager student.

4 References

- Hayes, J. F.** , W. G. Hill. 1981. Modification of estimates of parameters in the construction of genetic selection indices (‘bending’). *Biometrics* 37:483-493.
- Jorjani, H.** , L. Klei, U. Emanuelson. 2003. A simple method for weighted bending of genetic (co)variance matrices. *J. Dairy Sci.* 86:677-679.
- Meyer, K.** , M. Kirkpatrick. 2010. Better estimates of genetic covariance matrices by “bending” using penalized maximum likelihood. *Genetics* 185:1097-1110.