# Basic concepts in matrix algebra

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2022-03-10

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#### 1 Derivation of mean and variance of quadratic forms

This appendix supplies some general matrix algebra that is useful in these notes. Proof of these, as well as additional explanation, can be found in e.g. Searle [1982], Searle et al. [1992] and/or Knight [2008]. And Schaeffer's EuropeNotes p. 194.

The matrix V is the square variance-covariance matrix V = ZGZ' + D.

Denoting the derivative of the matrix:

$$\mathbf{V}_{i} = \frac{\partial \mathbf{V}}{\partial \sigma_{i}^{2}} = \begin{cases} \mathbf{D}_{n} & \text{when } \sigma_{i}^{2} = \sigma_{e}^{2} \\ \mathbf{ZGZ'} & \text{when } \sigma_{i}^{2} = \sigma_{g}^{2} \end{cases}$$
(1)

 $\mathbf{3}$ 

The derivative of the first quadratic from with respect to X:

$$\frac{\partial (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})' \mathbf{V} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})}{\partial \mathbf{X}} = -2\mathbf{X}' \mathbf{V} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$
(2)

The derivative of the *inverse* matrix

$$\frac{\partial \mathbf{V}^{-1}}{\partial \sigma_i^2} = -\mathbf{V}^{-1} \mathbf{V}_i \mathbf{V}^{-1} \tag{3}$$

The derivative of the trace of the matrix

$$\frac{\partial \operatorname{Tr}(\mathbf{V})}{\partial \sigma_i^2} = \operatorname{Tr}(\mathbf{V}_i) \tag{4}$$

The derivative of the logarithm of the matrix' determinant:

$$\frac{\partial \ln |\mathbf{V}|}{\partial \sigma_i^2} = \text{Tr}(\mathbf{V}^{-1}\mathbf{V}_i) \tag{5}$$

The derivative of the first and second quadratic forms, when taken with respect to  $\sigma_i^2$ :

$$\frac{\partial (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})' \mathbf{V} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})}{\partial \sigma_i^2} = (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})' \mathbf{V}_i (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$
(6a)

$$\frac{\partial (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})' \mathbf{V}^{-1} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})}{\partial \sigma_i^2} = -(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})' \mathbf{V}^{-1} \mathbf{V}_i \mathbf{V}^{-1} (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$
(6b)

and the derivative of the logarithm of the determinant of the second quadratic form:

$$\frac{\partial \ln |\mathbf{X}'\mathbf{V}^{-1}\mathbf{X}|}{\partial \sigma_i^2} = \text{Tr}((\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1}\mathbf{V}_i\mathbf{V}^{-1}\mathbf{X})$$
(6c)

but also [Knight, 2008, p. 21]:

$$\begin{split} &\frac{\partial \ln |\mathbf{V}|}{\partial \sigma_i^2} + \frac{\partial \ln |\mathbf{X}'\mathbf{V}^{-1}\mathbf{X}|}{\partial \sigma_i^2} \\ &= \mathrm{Tr}(\mathbf{V}^{-1}\mathbf{V}_i) - \mathrm{Tr}((\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1}\mathbf{V}_i\mathbf{V}^{-1}\mathbf{X}) \\ &= \mathrm{Tr}(\mathbf{V}^{-1}\mathbf{V}_i - (\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1}\mathbf{V}_i\mathbf{V}^{-1}\mathbf{X}) \\ &= \mathrm{Tr}(\mathbf{P}\mathbf{V}_i). \end{split}$$

A projection matrix, P can be defined as

$$P = V^{-1} - V^{-1}X(X'V^{-1}X)^{-1}X'V^{-1}$$
(7)

% and has following nice properties:

$$\mathbf{PX} = 0 \tag{8}$$

$$\mathbf{P}\mathbf{y} = \mathbf{V}^{-1}(\mathbf{y} - \mathbf{X}\hat{\boldsymbol{\beta}}), \text{ where}$$
 (9)

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1}\mathbf{y} \tag{10}$$

$$\hat{\mathbf{P}}\mathbf{y} = \hat{\mathbf{e}} \tag{11}$$

The derivative of the projection matrix:

$$\frac{\partial \mathbf{P}}{\partial \sigma_i^2} = -\mathbf{P} \mathbf{V}_i \mathbf{P} \tag{12}$$

For traces, we have:

$$Tr(\mathbf{P}) = \mathbf{y}'\mathbf{P}\mathbf{P}\mathbf{y} \tag{13a}$$

or

$$Tr(\mathbf{PV}_i) = \mathbf{y}' \mathbf{PV}_i \mathbf{Py}. \tag{13b}$$

%

### Some forms

In (??) on page ??, the form  $\mathbf{ZGZ}'$  is used. The following is the result if we consider a very simple example with two animals, where the first has two observations and the second only one.

$$\mathbf{y} = \mu + \mathbf{Z}\mathbf{g} + \mathbf{e}$$

$$\mathbf{Z} = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\mathbf{G} = \begin{bmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{bmatrix}$$

$$\mathbf{Z}\mathbf{G}\mathbf{Z}' = \begin{bmatrix} g_{11} & g_{11} & g_{12} \\ g_{11} & g_{11} & g_{12} \\ g_{21} & g_{22} \end{bmatrix}$$

$$\mathbf{Z}\mathbf{Z}' = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$
(14)

## 1 Derivation of mean and variance of quadratic forms

If we assume that  $\mathbf{y} \sim N(\mu, \mathbf{V})$  then [Searle et al., 1992, p. 466]

$$E(\mathbf{y}'\mathbf{Q}\mathbf{y}) = \text{Tr}(\mathbf{Q}\mathbf{V}) + \mu'\mathbf{Q}\mu$$
$$\text{Var}(\mathbf{y}'\mathbf{Q}\mathbf{y}) = 2 \text{Tr}(\mathbf{Q}\mathbf{V}\mathbf{Q}\mathbf{V}) + 4\mu'\mathbf{Q}\mathbf{V}\mathbf{Q}\mu$$

The quadratic form  $\mathbf{y}'\mathbf{Q}\mathbf{y}$  has a non-central  $\chi^2$  distribution with  $rank(\mathbf{Q})$  degrees of freedom and non-central parameter  $\frac{1}{2}\mu'\mathbf{Q}\mu$ , if and only if  $\mathbf{Q}\mathbf{V}$  is idempotent (Theorem S2, p. 467, Searle et al., 1992). When  $\mathbf{Q}\mathbf{V}$  is idempotent, then  $\mathbf{Q}\mathbf{V}\mathbf{Q}\mathbf{V} = \mathbf{Q}\mathbf{V} \Rightarrow \text{Tr}(\mathbf{Q}\mathbf{V}\mathbf{Q}\mathbf{V}) = \text{Tr}(\mathbf{Q}\mathbf{V})$ , and  $\text{Tr}(\mathbf{Q}\mathbf{V}) = rank(\mathbf{Q}\mathbf{V})$ .

Because  $\mu = 0$ ,  $\mathbf{V} = \mathbf{I}$ , and  $\mathbf{Q} = \mathbf{V}_0^{\frac{1}{2}} \mathbf{M} \mathbf{V}_0^{\frac{1}{2}}$  (where  $\mathbf{M} = \mathbf{V}_0^{-1} \mathbf{Z} \mathbf{G}_i \mathbf{Z}' \mathbf{V}_0^{-1}$ ), the expectation and variance of the quadratic form are

$$E(\mathbf{y}'\mathbf{Q}\mathbf{y}) = \text{Tr}(\mathbf{Q})$$

$$= \text{Tr}\left(\frac{1}{2}\mathbf{V}_0^{\frac{1}{2}}\mathbf{V}_0^{-1}\mathbf{Z}\mathbf{G}_i\mathbf{Z}'\mathbf{V}_0^{-1}\mathbf{V}_0^{\frac{1}{2}}\right)$$

$$= \frac{1}{2}\text{Tr}\left(\mathbf{V}_0^{\frac{1}{2}}\mathbf{V}_0^{-1}\mathbf{Z}\mathbf{G}_i\mathbf{Z}'\mathbf{V}_0^{-1}\mathbf{V}_0^{\frac{1}{2}}\right)$$

$$= \frac{1}{2}\text{Tr}\left(\mathbf{V}_0^{-1}\mathbf{Z}\mathbf{G}_i\mathbf{Z}'\right)$$

and

$$Var(\mathbf{y}'\mathbf{Q}\mathbf{y}) = 2 \operatorname{Tr}(\mathbf{Q}\mathbf{Q})$$

$$= 2 \operatorname{Tr}\left(\left[\frac{1}{2}\mathbf{V}_{0}^{\frac{1}{2}}\mathbf{V}_{0}^{-1}\mathbf{Z}\mathbf{G}_{i}\mathbf{Z}'\mathbf{V}_{0}^{-1}\mathbf{V}_{0}^{\frac{1}{2}}\right] \left[\frac{1}{2}\mathbf{V}_{0}^{\frac{1}{2}}\mathbf{V}_{0}^{-1}\mathbf{Z}\mathbf{G}_{i}\mathbf{Z}'\mathbf{V}_{0}^{-1}\mathbf{V}_{0}^{\frac{1}{2}}\right]\right)$$

$$= \frac{1}{2} \operatorname{Tr}\left(\left[\mathbf{V}_{0}^{\frac{1}{2}}\mathbf{V}_{0}^{-1}\mathbf{Z}\mathbf{G}_{i}\mathbf{Z}'\mathbf{V}_{0}^{-1}\mathbf{V}_{0}^{\frac{1}{2}}\right] \left[\mathbf{V}_{0}^{\frac{1}{2}}\mathbf{V}_{0}^{-1}\mathbf{Z}\mathbf{G}_{i}\mathbf{Z}'\mathbf{V}_{0}^{-1}\mathbf{V}_{0}^{\frac{1}{2}}\right]\right)$$

$$= \frac{1}{2} \operatorname{Tr}\left(\mathbf{V}_{0}^{-1}\mathbf{Z}\mathbf{G}_{i}\mathbf{Z}'\mathbf{V}_{0}^{-1}\mathbf{Z}\mathbf{G}_{i}\mathbf{Z}'\mathbf{V}_{0}^{-1}\mathbf{V}_{0}^{\frac{1}{2}}\mathbf{V}_{0}^{\frac{1}{2}}\right)$$

$$= \frac{1}{2} \operatorname{Tr}\left(\mathbf{V}_{0}^{-1}\mathbf{Z}\mathbf{G}_{i}\mathbf{Z}'\mathbf{V}_{0}^{-1}\mathbf{Z}\mathbf{G}_{i}\mathbf{Z}'\right).$$

We can further elaborate that  $\mathbf{y}'\mathbf{Q}\mathbf{y}$  is  $\chi^2$  distributed with  $\text{Tr}(\mathbf{Q})$  degrees of freedom under the conditions above.

#### References

Emma Knight. Improved Iterative Schemes for REML Estimation of Variance Parameters in Linear Mixed Models. Phd thesis, School of Agriculture, Food and Wine, University of Adelaide, 2008.

Shayle R. Searle. *Matrix Algebra Useful for Statistics*. Wiley Series in Probability and Statistics. John Wiley & Sons, Hoboken, New Jersey, 1st edition, 1982. ISBN 978-0-470-00961-1. Reprinted in 2006.

Shayle R. Searle, George Casella, and Charles E. McCulloch. *Variance Components*. Wiley Series in Probability and Statistics. John Wiley & Sons, Hoboken, New Jersey, 1992. ISBN 978-0-470-00959-8. Reprinted in 2006.