



ECONOMICS

ON THE DIFFERENTIATION OF A LOG-LIKELIHOOD FUNCTION USING MATRIX CALCULUS

by

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Business School The University of Western Australia

DISCUSSION PAPER 11.06

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ABSTRACT

Simple theorems based on a mathematical property of $\frac{\partial \text{vec}Y}{\partial \text{vec}X}$ provide powerful tools for obtaining matrix calculus results. By way of illustration, new results are obtained for matrix derivatives involving vecA, vechA, v(A) and vecX where X is a symmetric matrix. The analysis explains exactly how a log-likelihood function should be differentiated using matrix calculus.

Keywords: Matrix Derivatives, Vecs, Log-Likelihood Function

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<u>1.</u> <u>Introduction¹</u>

In a recent article Magnus (2010) advocates $\frac{\partial \text{vec}Y}{\partial \text{vec}X'}$ as the concept of the matrix derivative to use for the differentiation of a matrix Y with respect to the matrix X. He does this on the grounds of mathematical correctness and mathematical convenience. As far as the first ground is concerned, Parring (1992) shows that the three concepts of the matrix derivative of Y with respect to X, commonly used in the literature, all qualify as permissible mathematical operators. It depends on the matrix or vector space you are working with and how this space is normed. (For relationships that exist between these three concepts see Turkington (2007)). However, I would agree with Magnus on the second ground. Certainly $\frac{\partial \text{vec}Y}{\partial \text{vec}X'}$ is the most convenient concept of a matrix derivative to work with out of the concepts he considers. Having said that, an argument can be made for working with $\frac{\partial \text{vec}Y}{\partial \text{vec}X}$, which is just the

transpose of the concept advocated by Magnus. But this transpose makes a difference in terms of mathematical convenience.

In the next section it will be explained as succinctly as possible why from a practitioner's point of view $\frac{\partial \text{vec}Y}{\partial \text{vec}X}$ has certain mathematical advantages over all the other concepts of matrix derivatives used in the literature. Simple theorems involving this concept will be presented, whose proofs are almost trivial. However, taken together, these theorems provide powerful tools for deriving matrix calculus results.

This is demonstrated both in section 3 and section 4 of the article. In section 3 use is made of these theorems to derive results, some of which are new, for derivatives involving vecA,

vechA and $\overline{v}(A)$ where A is a square matrix. These three vectors are of interest to statisticians. In section 4 the same theorems are used to derive an easy method for obtaining derivatives involving the vecs of symmetric matrices from known matrix calculus results. Again this is of interest to statisticians as covariance matrices appear in log-likelihood functions.

Section 5 brings the analysis together and demonstrates how matrix calculus should be used to correctly differentiate a log-likelihood function. The last section is reserved for a brief conclusion.

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<u>2.</u> Theorems involving $\partial \text{vecY} / \partial \text{vecX}$

The main advantage of using this concept of a matrix derivative can be put succinctly in a few lines. Consider a $m \times 1$ vector $y = (y_1 \dots y_m)'$, a $n \times 1$ vector $x = (x_1 \dots x_n)'$ and ℓ any scalar function. Then using $\frac{\partial \operatorname{vec} Y}{\partial \operatorname{vec} X}$ as our concept of a matrix derivative

$$\frac{\partial \ell}{\partial y} = \left(\frac{\partial \ell}{\partial y_1} \quad \dots \quad \frac{\partial \ell}{\partial y_m}\right)' \text{ and } \frac{\partial \ell}{\partial x} = \left(\frac{\partial \ell}{\partial x_1} \quad \dots \quad \frac{\partial \ell}{\partial x_n}\right)'. \text{ Suppose } y = Ax \text{, where A is a matrix of}$$

constants, that is, the elements of A are not scalar functions of x. Then,

$$\frac{\partial \ell}{\partial y} = A \frac{\partial \ell}{\partial x},$$

so for this important case the same functional relation exists between $\frac{\partial \ell}{\partial y}$ and $\frac{\partial \ell}{\partial x}$ as between y and x.

Several of the following theorems involving $\frac{\partial \text{vec}Y}{\partial \text{vec}X}$ arise from this notion.

Theorem 1

Let x be a $n \times 1$ vector whose elements are distinct. Then

$$\frac{\partial \mathbf{X}}{\partial \mathbf{x}} = \mathbf{I}_{\mathrm{n}} \,.$$

Proof

Clearly

$$\frac{\partial x}{\partial x} = \begin{pmatrix} \frac{\partial x_1}{\partial x} & \dots & \frac{\partial x_n}{\partial x} \end{pmatrix} = \begin{pmatrix} e_1^n & \dots & e_n^n \end{pmatrix} = I_n \quad ,$$

where e_j^n is the jth column of I_n .

Theorem 2

Suppose x and y are two column vectors and y = Ax where A is a matrix of constants.

Let z be a column vector. Then

$$\frac{\partial z}{\partial y} = A \frac{\partial z}{\partial x} \quad .$$

Proof

We know that for any scalar ℓ ,

$$\frac{\partial \ell}{\partial y} = A \frac{\partial \ell}{\partial x} \quad .$$

Write

$$\mathbf{z} = \begin{pmatrix} z_1 & \dots & z_p \end{pmatrix}' \quad .$$

Then

$$\frac{\partial z}{\partial y} = \left(\frac{\partial z_1}{\partial y} \quad \dots \quad \frac{\partial z_p}{\partial y}\right) = \left(A\frac{\partial z_1}{\partial x} \quad \dots \quad A\frac{\partial z_p}{\partial x}\right) = A\left(\frac{\partial z_1}{\partial x} \quad \dots \quad \frac{\partial z_p}{\partial x}\right) = A\frac{\partial z}{\partial x} \quad .$$

Theorem 3

Suppose x and y are two column vectors such that

y = Ax

where A is a matrix of constants and the elements of x are distinct. Then

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \left(\frac{\partial \mathbf{x}}{\partial \mathbf{y}}\right)'$$

.

Proof

Using the advocated concept of a matrix derivative $\frac{\partial y}{\partial x} = A'$. But from theorem 2

$$\frac{\partial z}{\partial y} = A \frac{\partial z}{\partial x}$$

for any vector z. Taking z = x gives

$$\frac{\partial x}{\partial y} = A \frac{\partial x}{\partial x}$$

and as the elements of x are distinct by theorem 1, the derivative $\frac{\partial x}{\partial x}$ is the identity matrix so

$$\frac{\partial \mathbf{x}}{\partial \mathbf{y}} = \mathbf{A} = \left(\frac{\partial \mathbf{y}}{\partial \mathbf{x}}\right)'.$$

Taking transposes gives the result.

In using the recommended concept of a matrix derivative a backward chain rule applies (see Turkington (2004)) which is just the transpose of the chain rule reported by Magnus (see Magnus (2010)). That is, if y is a vector function of u and u is a vector function of x, so y = y(u(x)) then

$$\partial y = \frac{\partial u \, \partial y}{\partial x \, \partial u}$$
 .

Using this result gives us the following theorem.

Theorem 4

For any vectors x and y

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \frac{\partial \mathbf{x} \, \partial \mathbf{y}}{\partial \mathbf{x} \, \partial \mathbf{x}}$$

•

Proof

Write y = y(x(x)) and apply the backward chain rule.

* * * *

3. Theorems concerning derivatives involving vecA, vechA and $\overline{v}(A)$

Let $A = \{a_{ij}\}$ be a $n \times n$ matrix and partition A into its columns so $A = (a_1 \dots a_n)$ where a_j is the jth column of A for $j = 1, \dots, n$. Then vecA is the $n^2 \times 1$ vector given by

 $\operatorname{vecA} = \begin{pmatrix} a_1' & \dots & a_n' \end{pmatrix}'$, that is, to form vecA we stack the columns of A underneath each other. VechA is the $\frac{1}{2}n(n+1) \times 1$ vector given by

$$\operatorname{vechA} = (a_{11} \dots a_{n1} \ a_{22} \dots \ a_{n2} \ \dots \ a_{nn})'$$

That is, to form vechA we stack the elements of A on and below the main diagonal one underneath the other. The vector $\overline{v}(A)$ is the is the $\frac{1}{2}n(n-1)\times 1$ vector given by

$$v(A) = (a_{11} \dots a_{n1} a_{32} \dots a_{n2} \dots a_{nn-1})'$$

That is, we form v(A) by stacking the elements of A below the main diagonal, one beneath the other. These vectors are important for statisticians and econometricians. If A is a covariance matrix then vecA contains the variances and covariances but with the covariances duplicated. The vector vechA contains the variances and covariances without duplication and v(A) contains the covariances without the variances.

Regardless as to whether A is symmetric or not, the elements in vechA and v(A) are distinct. The elements in vecA are distinct provided A is not symmetric. If A is symmetric the elements of vecA are not distinct. So from theorem 1 we have

$$\frac{\partial \text{vechA}}{\partial \text{vechA}} = I_{\frac{1}{2}n(n+1)} \qquad \text{for all A}$$

$$\frac{\partial \overline{v}(A)}{\partial \overline{v}(A)} = I_{\frac{1}{2}n(n-1)} \qquad \text{for all A}$$

$$\frac{\partial \text{vecA}}{\partial \text{vecA}} = I_{n^2} \qquad \text{provided A is not symmetric.}$$

What
$$\frac{\partial \text{VecA}}{\partial \text{vecA}}$$
 is in the case where A symmetric is discussed in section 4.

Regardless of the nature of A, it is well known that there exist $\frac{1}{2}n(n+1) \times n^2$ and $\frac{1}{2}n(n-1) \times n^2$ zero-one matrices L_n and \overline{L}_n respectively, such that

$$L_n vec A = vec h A$$

and

$$L_n \operatorname{vec} A = v(A)$$

If A is symmetric then

$$N_n vec A = vec A$$

where $N_n = \frac{1}{2}(I_{n^2} + K_{nn})$ and K_{nn} is a commutation matrix, so for this case

$$L_n N_n \text{vec} A = \text{vech} A$$

and

$$\overline{L}_n$$
NvecA = $\overline{v}(A)$.

The matrices $L_n N_n$ and $\overline{L}_n N_n$ are not zero-one matrices. However, along with L_n and \overline{L}_n , they form a group of matrices known as elimination matrices. The difference in the operation of L_n and $L_n N_n$ on vecA is this. The matrix L_n chooses a_{ij} for i > j for vechA directly from vecA,

whereas $L_n N_n$ recognises that A is symmetric and forms a_{ij} for vechA using $a_{ij} = \frac{a_{ij} + a_{ji}}{2}$.

For special cases there exist zero-one matrices called duplication matrices which take us back from vechA and $\overline{v}(A)$ to vecA. If A is symmetric there exists a $n^2 \times \frac{1}{2}n(n+1)$ zero-one matrix D_n such that

$$D_n \operatorname{vech} A = \operatorname{vec} A$$
.

If A is strictly lower triangular then

$$\overline{L}_n'\overline{v}(A) = \operatorname{vec} A$$
.

For an excellent discussion of the special matrices associated with vecA, vechA and $\overline{v}(A)$ and their properties see Magnus (1988).

Consider ℓ any scalar function. Then the same relationships exist between $\frac{\partial \ell}{\partial \text{vecA}}$, $\frac{\partial \ell}{\partial \text{vechA}}$ and $\frac{\partial \ell}{\partial \ell}$ as exist between vecA, vechA and $\overline{v}(A)$ respectively.

and $\frac{\partial \ell}{\partial \overline{v}(A)}$ as exist between vecA, vechA and $\overline{v}(A)$ respectively.

Thus for general A

$$\frac{\partial \ell}{\partial \text{vechA}} = L_n \frac{\partial \ell}{\partial \text{vecA}}$$
$$\frac{\partial \ell}{\partial \overline{v}(A)} = \overline{L}_n \frac{\partial \ell}{\partial \text{vecA}}$$

For symmetric A

$$\frac{\partial \ell}{\partial \text{vechA}} = L_n N_n \frac{\partial \ell}{\partial \text{vecA}}$$
(1)
$$\frac{\partial \ell}{\partial \overline{v}(A)} = \overline{L}_n N_n \frac{\partial \ell}{\partial \text{vecA}} .$$

$$\frac{\partial \ell}{\partial \text{vecA}} = D_n \frac{\partial \ell}{\partial \text{vechA}}$$

.

and for A a strictly lower triangular matrix

$$\frac{\partial \ell}{\partial \text{vecA}} = \overline{L}_n' \frac{\partial \ell}{\partial \overline{v}(A)}$$

Using the theorems of section 3 we can prove the following results.

Theorem 5

$$\frac{\partial \text{vecA}}{\partial \text{vechA}} = \mathbf{D}_n' \qquad \text{if A is symmetric}$$
$$\frac{\partial \text{vecA}}{\partial \text{vechA}} = \mathbf{L}_n \qquad \text{if A is not symmetric.}$$

Proof

If A is symmetric $vecA = D_n vechA$ and the result follows. For the case where A is not symmetric consider

$$vechA = L_n vecA$$
.

By theorem 2 we have that for any vector z

$$\frac{\partial z}{\partial \text{vechA}} = L_n \frac{\partial z}{\partial \text{vecA}} \ .$$

Taking z = vecA gives

$$\frac{\partial \text{vecA}}{\partial \text{vechA}} = L_n \frac{\partial \text{vecA}}{\partial \text{vecA}}$$

and as A is not symmetric the elements of vecA are distinct, so by theorem 1

$$\frac{\partial \text{vecA}}{\partial \text{vecA}} = \mathbf{I}_{n^2}$$

and

$$\frac{\partial \text{vecA}}{\partial \text{vechA}} = L_n \,.$$

* * * *

Theorem 6

$$\frac{\partial \text{vechA}}{\partial \text{vecA}} = D_n \qquad \text{if A is symmetric}$$
$$\frac{\partial \text{vechA}}{\partial \text{vecA}} = L_n' \qquad \text{if A is not symmetric.}$$

Proof

A trivial application of theorem 3.

* * * *

The method used in theorem 5 can also be used to quickly derive results about elimination matrices, duplication matrices and the matrix N_n . Consider for example the case where A is a symmetric $n \times n$ matrix so

$$L_n N_n \text{vec} A = \text{vech} A$$
.

By theorem 2 for any vector z

$$\frac{\partial z}{\partial \text{vechA}} = L_n N_n \frac{\partial z}{\partial \text{vecA}} \quad .$$

Take z = vechA. Then

$$\frac{\partial \text{vechA}}{\partial \text{vechA}} = L_n N_n \frac{\partial \text{vechA}}{\partial \text{vecA}} = L_n N_n D_n$$

by theorem 6.

But as the elements of vechA are distinct

$$\frac{\partial \text{vechA}}{\partial \text{vechA}} = \mathbf{I}_{\frac{1}{2}^{n(n+1)}},$$

so

$$L_n N_n D_n = I_{\frac{1}{2}n(n+1)}$$
 (2)

4. Theorems concerning derivatives involving vecX where X is symmetric

Consider X a $n \times n$ symmetric matrix and let x = vecX. Then the elements of x are not distinct and one of the implications of this is that

$$\frac{\partial x}{\partial x} \neq I_{n^2}$$

.

Consider the 2×2 case. Then

$$\mathbf{X} = \begin{pmatrix} \mathbf{X}_{11} & \mathbf{X}_{21} \\ \mathbf{X}_{21} & \mathbf{X}_{22} \end{pmatrix}$$

and $\mathbf{x} = \begin{pmatrix} x_{11} & x_{21} & x_{21} & x_{22} \end{pmatrix}'$, so

$$\frac{\partial \mathbf{x}}{\partial \mathbf{x}} = \begin{pmatrix} \frac{\partial \mathbf{x}_{11}}{\partial \mathbf{x}} & \frac{\partial \mathbf{x}_{21}}{\partial \mathbf{x}} & \frac{\partial \mathbf{x}_{21}}{\partial \mathbf{x}} & \frac{\partial \mathbf{x}_{22}}{\partial \mathbf{x}} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Clearly this matrix is not the identity matrix. What it is, is given by the following theorem whose proof again calls on our results of section 3.

Theorem 7

Let X be a $n \times n$ symmetric matrix. Then

$$\frac{\partial \text{vec}X}{\partial \text{vec}X} = D_n D_n'$$

Proof

As X is a n×n symmetric matrix

 $vecX = D_n vechX$

so it follows from theorem 2 that for any vector z

$$\frac{\partial z}{\partial \text{vec} X} = D_n \frac{\partial z}{\partial \text{vech} X}$$

Take z = vecX so

$$\frac{\partial \text{vec}X}{\partial \text{vec}X} = D_n \frac{\partial \text{vec}X}{\partial \text{vech}X} = D_n D_n'$$
(3)

.

•

by theorem 5.

The fact that in the case where X is a $n \times n$ symmetric matrix $\frac{\partial \text{vecX}}{\partial \text{vecX}} = D_n D_n'$ means that all

the usual rules of matrix calculus, regardless of what concept of a matrix derivative one is using, do not apply for vecX where X is symmetric. However theorem 4, coupled with theorem 7, provides a quick and easy method for finding the results for this case using known matrix calculus results. Consider again x = vecX with X a symmetric matrix. Let $\frac{\phi y}{\phi x}$ denote the matrix derivative we would get if we differentiated y with respect to x using the concept of differentiation advocated but *ignoring the fact that X is a symmetric matrix*. Then the full import of theorem 4 for this case is given by the equation

$$\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \frac{\partial \mathbf{x} \, \phi \mathbf{y}}{\partial \mathbf{x} \, \phi \mathbf{x}} \quad . \tag{4}$$

Combining Eqs. (3) and (4) give the following theorem.

Theorem 8

Consider y = y(x) with x = vecX and X is a $n \times n$ symmetric matrix. Let $\frac{\phi y}{\phi x}$ denote the

derivative of y with respect to x obtained when we ignore the fact that X is a symmetric matrix. Then

_

$$\frac{\partial y}{\partial x} = D_n D_n' \frac{\phi y}{\phi x} \quad . \tag{5}$$

A few examples will suffice to illustrate the use of this theorem. (For the rules referred to in these examples see Turkington (2004), Lutkepohl (1996) or Magnus and Neudecker (1999)).

For x with distinct elements and A a matrix of constants we know that

*

$$\frac{\partial \mathbf{x}' \mathbf{A} \mathbf{x}}{\partial \mathbf{x}} = 2(\mathbf{A} + \mathbf{A}')\mathbf{x}$$

•

It follows that when x = vecX and X is a $n \times n$ symmetric matrix

$$\frac{\partial x'Ax}{\partial x} = 2D_n D_n'(A + A')x$$

For X non-singular but non-symmetric matrix

$$\frac{\partial |\mathbf{X}|}{\partial \operatorname{vec} \mathbf{X}} = |\mathbf{X}| \operatorname{vec}(\mathbf{X}^{-1})'$$

so for X non-singular but symmetric

$$\frac{\partial |\mathbf{X}|}{\partial \operatorname{vec} \mathbf{X}} = |\mathbf{X}| \mathbf{D}_{n} \mathbf{D}_{n}' \operatorname{vec} \mathbf{X}^{-1}$$

For X a n×n non-symmetric matrix, A and B matrices of constants

$$\frac{\partial \text{vecAXB}}{\partial \text{vecX}} = \mathbf{B} \otimes \mathbf{A}'$$

so for X a $n \times n$ symmetric matrix

$$\frac{\partial \text{vecAXB}}{\partial \text{vecX}} = D_n D_n'(B \otimes A')$$

All results using either $\frac{\partial \text{vec}Y}{\partial \text{vec}X}$ or $\frac{\partial \text{vec}Y}{\partial \text{vec}X'}$ (in which case we have to take transposes) can be adjusted in this way to allow for the case where X is a symmetric matrix.

5. <u>The Matrix Differentiation of a Log-Likelihood Function.</u>

Suppose we are dealing with a statistical model that has a log-likelihood function $\ell(\theta)$ where θ is a vector containing the parameters of the model. Then we can always partition θ as $\theta = (\delta' v')'$ where $v = \text{vech}\Sigma$ and Σ is a covariance matrix associated with the model. The problem is that $\ell(\theta)$ is never expressed in terms of v. Rather it is written in terms of Σ . The question then is how do we form $\frac{\partial \ell}{\partial v}$. The results of the previous section allow us to do this. As Σ is a symmetric matrix and assuming it is $n \times n$ we have from theorem 8 that

$$\frac{\partial \ell}{\partial \text{vec}\Sigma} = \mathbf{D}_{n} \mathbf{D}_{n}' \frac{\phi \ell}{\phi \text{vec}\Sigma}$$

But from Eq. (1) we also have

$$\frac{\partial \ell}{\partial v} = L_n N_n \frac{\partial \ell}{\partial vec \Sigma}$$

so

$$\frac{\partial \ell}{\partial v} = L_n N_n D_n D_n' \frac{\phi \ell}{\phi \text{vec} \Sigma} = D_n' \frac{\phi \ell}{\phi \text{vec} \Sigma}$$

as by Eq. (2) $L_n N_n D_n = I_{\frac{1}{2}n(n+1)}$. Our method then is to differentiate the log likelihood function with respect to vec Σ ignoring the fact that Σ is symmetric. Then premultiply the result by D_n' . Note that from theorem 5, $\frac{\partial \text{vec}\Sigma}{\partial y} = D_n'$ so we could write if we like that

$$\frac{\partial \ell}{\partial v} = \frac{\partial \text{vec}\Sigma \quad \phi \ell}{\partial v \quad \phi \text{vec}\Sigma}$$

which resembles a backward chain rule. This is approach was taken by Turkington (2004).

A simple example illustrates this method. Magnus and Neudecker (1980) consider a sample of size m from a n dimensional distribution of a random vector y with mean vector μ and a positive definite covariance matrix Σ . The parameters of this model are $\theta = (\mu' v')'$ where $v = \text{vech}\Sigma$ and the log likelihood function, apart from a constant, is

$$\ell(\theta) = -\frac{1}{2} \mathrm{mlog} |\Sigma| - \frac{1}{2} \mathrm{tr} \Sigma^{-1} Z$$

where

$$Z = \sum_{i=1}^{m} (y_i - \mu)(y_i - \mu)'$$

Now

$$\frac{\phi \ell}{\phi \text{vec}\Sigma} = -\frac{1}{2} m \frac{\phi \text{log}\Sigma}{\phi \text{vec}\Sigma} - \frac{1}{2} \frac{\phi}{\phi \text{vec}\Sigma} \text{tr}\Sigma^{-1} Z$$

and

$$\frac{\phi \mathrm{log}\Sigma}{\phi \mathrm{vec}\Sigma} = \mathrm{vec}\Sigma^{-1}$$

Using the backward chain rule

$$\frac{\phi \text{tr} \Sigma^{-1} Z}{\phi \text{vec} \Sigma} = \frac{\phi \text{vec} \Sigma^{-1} \phi \text{tr} \Sigma^{-1} Z}{\phi \text{vec} \Sigma \phi \text{vec} \Sigma^{-1}} = -(\Sigma^{-1} \otimes \Sigma^{-1}) \text{vec} Z$$

so

$$\frac{\phi\ell}{\phi \text{vec}\Sigma} = -\frac{1}{2}\text{mvec}\Sigma^{-1} + \frac{1}{2}(\Sigma^{-1}\otimes\Sigma^{-1})\text{vec}Z = \frac{1}{2}(\Sigma^{-1}\otimes\Sigma^{-1})\text{vec}(Z-m\Sigma)$$

 $\frac{\partial \ell}{\partial v} = \frac{1}{2} D'_{n} (\Sigma^{-1} \otimes \Sigma^{-1}) \operatorname{vec}(Z - m\Sigma)$

which is the same result Magnus and Neudecker obtained using differentials.

Conclusion

It goes without saying that the correct use of matrix calculus to differentiate a log likelihood function is of great interest to a statistician who wants to apply classical statistical procedures centred around the likelihood function. Once the method is understood using matrix calculus in these procedures, it is no more difficult than the use of ordinary calculus in every day mathematical problems. Moreover, there is no need to first resort to matrix differentials as advocated by Magnus and Neudecker (1999). Rather, using rules which are generalizations of the product rule and chain rule of ordinary calculus, one can easily derive the derivatives required in classical statistics using either $\frac{\partial \text{vec}Y}{\partial \text{vec}X'}$, as advocated by Magnus, or $\frac{\partial \text{vec}Y}{\partial \text{vec}X}$.

and

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