The Trace Function on Matrices

P. Reany

November 29, 2022

Abstract

In this paper, I present some properties of the trace function, which operates on square matrices. A basic knowledge matrices is assumed, and, in particular, that of the determinant of a matrix.

1 Introduction

This article will begin with the easy identities about the trace function and then progress to evermore difficult ones. But first, we need to define what is meant by the trace function of a square matrix.

Definition: In a square matrix A, the *main diagonal* starts at the upper left element a_{11} and proceeds down the diagonal to the lower right a_{nn}. See Fig. 1.

Definition: The elements of A not on the Main Diagonal are said to be 'off-diagonal' elements.

Definition: A square matrix is said to be 'diagonal' if its off-diagonal elements are all zero. Obviously, the zero matrix is trivially diagonal.

Definition: The symbol that will be used for the trace function in this paper is $\mathrm{Tr}\,()$. Thus, for the $n \times n$ matrix A,

$$\mathrm{Tr}\,(A) \equiv a_{11} + a_{22} + \cdots + \ a_{nn}\,, \tag{1}$$

that is, the trace is the sum of the components on the main diagonal.

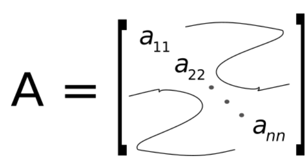

Figure 1. Let A be an $n \times n$ matrix. The 'diagonal elements' of A are those which begin at the top left and go in order to the bottom right. As depicted in the figure above, they are the elements $a_{11}, a_{22}, \ldots,\ a_{nn}$. The squiggly curves represent all the off-diagonal elements I'm ignoring for the moment.

Definition: The ordered set on the elements on the Main Diagonal of matrix A are presented in the convenient form $\mathrm{diag}\,(A) = (a_{11}, a_{22}, \ldots,\ a_{nn})$. (By the way, if the rows and columns start their counting at zero instead of at unity then $\mathrm{diag}\,(A) = (a_{00}, a_{11}, a_{22}, \ldots,\ a_{n-1n-1})$.) One advantage of introducing the diag() function is that it allows us to write down much more compact mathemtical expressions.

The diag() function is peculiar in that it can go the other way as well. Above, we put into its argument a matrix and received back the vector of its diagonal elements as its components. This time, we'll input a vector/array and output a diagonal matrix. Thus, for

$$v = v_1, v_2, \cdots , \ v_n \,, \tag{2}$$

then

$$\operatorname{diag}(v) = \begin{bmatrix} v_1 & & & \\ & v_2 & & \\ & & \ddots & \\ & & & v_n \end{bmatrix} , \tag{3}$$

where, this time, the voided entries are all zeros.

If we take the composition of diag functions, diag (diag (A)), we get back a diagonal matrix D, having on its main diagonal the diagonal elements of A. Thus, for

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} , \tag{4}$$

then $D = \operatorname{diag}(\operatorname{diag}(A)) = \operatorname{diag}^2(A)$, and

$$D = \begin{bmatrix} a_{11} & 0 & \cdots & 0 \\ 0 & a_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_{nn} \end{bmatrix} . \tag{5}$$

One last comment before we begin the identities. What kind of numbers can we allow as the components of the square matrices of interest to us? Well, for many purposes, we can allow them to be just elements of a ring, meaning that they won't need to have inverses. However, for the more advances requirements, we'll see later on, the nonzero elements will need inverses. So, let's just keep things simple and assume that the components are either from the real or complex numbers.

Definition: An $n \times n$ matrix whose trace is zero is said to be *traceless.* Now, in a traceless matrix the components on the main diagonal need not all be zero, but if they aren't, they need to add up to zero.

Definition: We define the Sum() function on a vector/linear-array of numbers. Let v be a vector/linear-array with n components $v_1, v_2, \ldots, v_n$. Then

$$\operatorname{Sum}(v) \equiv v_1 + v_2 + \cdots + v_n \,. \tag{6}$$

The following lemma

$$\operatorname{Tr}(AB) \neq \operatorname{Tr}(A)\operatorname{Tr}(B) \,, \tag{7}$$

is easy to prove, by way of providing a counterexample. Let

$$A = \begin{bmatrix} 1 & 1 \\ 0 & -1 \end{bmatrix} , \quad B = \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix} \quad \text{then} \quad AB = \begin{bmatrix} 2 & 1 \\ -1 & -1 \end{bmatrix} . \tag{8}$$

Then, $\operatorname{Tr}(A)\operatorname{Tr}(B) = 0 \cdot 2 = 0$, but $\operatorname{Tr}(AB) = 1$.

2 Simple identities of the Trace function

a) Let I_n be the $n \times n$ identity matrix. Then $\mathrm{Tr}\,(I_n) = n$. (Obvious.)

b) Let A^{t} stand for the transpose of A. Then $\mathrm{Tr}\,(A^{\mathrm{t}}) = \mathrm{Tr}\,(A)$. Since the transpose operation leaves the elements on the Main Diagonal fixed, this proof is obvious.

c) Let α be a scalar. Then $\mathrm{Tr}\,(\alpha A) = \alpha \mathrm{Tr}\,(A)$. To multiply a matrix by a scalar, one means that each element of the matrix is multiplied by the scalar. Thus,

$$\begin{aligned} \mathrm{diag}\,(\alpha A) &= (\alpha a_{11}, \alpha a_{22}, \ldots,\ \alpha a_{nn}) \\ &= \alpha(a_{11}, a_{22}, \ldots, a_{nn})\,. \end{aligned} \tag{9}$$

Now, $\mathrm{Tr}\,(\alpha A) = \mathrm{Tr}\,(\mathrm{diag}\,(\alpha A)) = \mathrm{Sum}(\mathrm{diag}\,(\alpha A)) = \alpha a_{11} + \alpha a_{22} + \cdots + \alpha a_{nn} = \alpha(a_{11} + a_{22} + \cdots + a_{nn})$. And, $\alpha \mathrm{Tr}\,(A) = \alpha \mathrm{Sum}(\mathrm{diag}\,(A)) = \alpha\,(a_{11} + a_{22} + \cdots + a_{nn})$. Hence, $\mathrm{Tr}\,(\alpha A) = \alpha \mathrm{Tr}\,(A)$.

d) Let A, B be $n \times n$ matrices. Then $\mathrm{Tr}\,(A + B) = \mathrm{Tr}\,(A) + \mathrm{Tr}\,(B)$. We begin with the fact that matrices are added together component-wise, so that the i, jth component of $(A+B)_{ij} = A_{ij} + B_{ij}$. Therefore the ith component on the main diagonal of this sum is $A_{ii} + B_{ii}$. Therefore,

$$\mathrm{Tr}\,(A + B) = \sum_{i=1}^{n} (A_{ii} + B_{ii})\,. \tag{10}$$

But,

$$\mathrm{Tr}\,(A) + \mathrm{Tr}\,(B) = \sum_{i=1}^{n} A_{ii} + \sum_{i=1}^{n} B_{ii} = \sum_{i=1}^{n} (A_{ii} + B_{ii})\,. \tag{11}$$

Hence, $\mathrm{Tr}\,(A + B) = \mathrm{Tr}\,(A) + \mathrm{Tr}\,(B)$. Corollary: $\mathrm{Tr}\,(A - B) = \mathrm{Tr}\,(A) - \mathrm{Tr}\,(B)$.

e) Let A, B be $n \times n$ matrices. Then $\mathrm{Tr}\,(AB) = \mathrm{Tr}\,(BA)$. The proof of this is not too difficult. The method is to look at the diagonal elements of both AB and BA by multiplying them together in indice form and then show that $\mathrm{diag}\,(AB) = \mathrm{diag}\,(BA)$. It's trivial from there.

f) Let $[\,A, B\,]$ be the commutator of A and B, where $[\,A, B\,] \equiv AB - BA$. Show that $\mathrm{Tr}\,([\,A, B\,]) = 0$. This result follows trivially as a corollary to the last lemma.

g) Let $A_1, A_2, \ldots, A_k$ be k $n \times n$ matrices. Then

$$\mathrm{Tr}\,(A_1 A_2 \cdots A_k) = \mathrm{Tr}\,(A_2 \cdots A_k A_1)\,. \tag{12}$$

In essence, we've cyclically permuted the left-most factor to the right side of the product. The proof of this involves induction. We need a base case to prove, which we can accept as proved by use of e), thus: $\mathrm{Tr}\,(A_1 A_2) = \mathrm{Tr}\,(A_2 A_1)$. Next, use the inductive hypothesis to assume that (12) is true for k factors and then prove that the relation (12) is true for $k \to k + 1$. Anticipating future needs, let's define $B = A_2 \cdots A_k A_{k+1}$, then

$$\begin{aligned} \mathrm{Tr}\,(A_1 A_2 \cdots A_k A_{k+1}) &= \mathrm{Tr}\,(A_1(A_2 \cdots A_k A_{k+1})) \\ &= \mathrm{Tr}\,(A_1 B) \\ &= \mathrm{Tr}\,(B A_1) \\ &= \mathrm{Tr}\,(A_2 \cdots A_k A_{k+1} A_1)\,. \end{aligned} \tag{13}$$

Since the relation held for case $k + 1$, the relation is assumed to be true for all $k \geq 2$. Now, we have shown that we can move the leftmost matrix all the way to the right, but we can also move the rightmost matrix all the way to the left by similar arguments.

Lemma 1 (for the next theorem)

Let A, D, P be $n \times n$ matrices, such that D is a diagonal matrix. Suppose further that P is invertible and that

$$A = P^{-1} D P\,. \tag{14}$$

Then $\mathrm{Tr}\,(A) = \mathrm{Tr}\,(D)$. We will use cyclic permutation of matrices in this proof.

Proof:

$$\mathrm{Tr}\,(A) = \mathrm{Tr}\,(P^{-1} D P) = \mathrm{Tr}\,(D P P^{-1}) = \mathrm{Tr}\,(D I) = \mathrm{Tr}\,(D)\,. \tag{15}$$

3 The Matrix Diagonalization Theorem

Now I want to employ a technique that can be found in Gilbert Strang's linear algebra textbook, *Linear Algebra for Everyone*,[1] pages 215–216.

Suppose A is an $n \times n$ matrix with n mutually orthonormal eigenvectors $\mathbf{x}_i$, each having corresponding eigenvalue λ_i. Then the following standard equation must be true for $k \in [\,1, 2, \ldots, n\,]$:

$$A\mathbf{x}_k = \lambda_k \mathbf{x}_k\,. \tag{16}$$

Now, since the RHS is a column vector, the LHS is too. Thus, we can make a new $n \times n$ matrix with n columns $A\mathbf{x}_i$, in which case, (16) generalizes to

$$[\,A\mathbf{x}_1\; A\mathbf{x}_2\; \ldots\; A\mathbf{x}_n\,] = [\,\lambda_1\mathbf{x}_1\; \lambda_2\mathbf{x}_2\; \ldots\; \lambda_n\mathbf{x}_n\,]\,. \tag{17}$$

However, this last equation is equivalent to

$$A\,[\,\mathbf{x}_1\, \mathbf{x}_2\; \ldots\; \mathbf{x}_n\,] = [\,\lambda_1\mathbf{x}_1\; \lambda_2\mathbf{x}_2\; \ldots\; \lambda_n\mathbf{x}_n\,]\,. \tag{18}$$

And this can be written more compactly as

$$A\,X = X\,\Lambda\,. \tag{19}$$

where

$$X \equiv [\,\mathbf{x}_1\, \mathbf{x}_2\; \ldots\; \mathbf{x}_n\,] \quad \text{and} \quad \Lambda \equiv \mathrm{diag}\,(\lambda_1, \lambda_2, \ldots, \lambda_n)\,. \tag{20}$$

Thus, X is an $n \times n$ matrix and Λ is an $n \times n$ diagonal matrix. Now, it's well-known that X is invertible, hence we can solve for Λ:

$$\Lambda = X^{-1} A\, X\,. \tag{21}$$

Therefore, we know from the last lemma that $\mathrm{Tr}\,(A) = \mathrm{Tr}\,(\Lambda)$, which is equal to the sum of the eigenvalues of A. Pretty neat!

Lemma 2 (some results without proof)

We need some result from the theory of determinants, such as, the fact that the determinant of a diagonal matrix is the product of the components on the main diagonal.

Let A, B be $n \times n$ matrices, then it is known that

$$\det(AB) = \det(A)\det(B)\,. \tag{22}$$

By induction, we can show that the determinant of a product of matrices is equal to the product of the determinant of the individual matrices, or

$$\det(A_1 A_2 \cdots A_k) = \det(A_1)\det(A_2)\cdots\det(A_k)\,. \tag{23}$$

Now, if A is invertible, $A^{-1}A = I$, then

$$\det(A^{-1}A) = \det(A^{-1})\det(A) = \det(I) = 1\,. \tag{24}$$

[1] G. Strang, *Linear Algebra for Everyone*, Wellesley-Cambridge Press, MA, USA (2020).

4 An advanced identity involving the Trace function

The next identity may look hard but it really isn't, so long as you understand how to take the exponential of a variable using the Taylor series. So, let's get that part out of the way now.

$$e^X \equiv \sum_{i=0}^{\infty} \frac{X^k}{k!}\,. \tag{25}$$

More commonly, the variable X is a real or complex number, but we will allow it to be an $n \times n$ matrix (why not?). Does (25) even make sense as a matrix equation? Let's see. The kth term on the RHS is

$$\frac{X^k}{k!}\,. \tag{26}$$

So, this tell us to multiply X by itself k times. That's a sensical matrix operation. Then we divide that result by $k!$. That's just dividing a matrix by a real number, so that makes sense. But how do we add together an infinite number of $n \times n$ matrices? We do that componentwise, and that also makes sense. Technically, we have to concern ourselves with whether or not each infinite sum converges, but we won't deal with that here.

So, here's our next theorem. Let A be an $n \times n$ diagonalizable matrix such that

$$A = P^{-1}DP\,, \tag{27}$$

where D is a diagonal matrix. Then,

$$\det e^{tX} = e^{t\,\mathrm{Tr}\,(A)}\,. \tag{28}$$

The t factor is just a scalar number. On the LHS we have the determinant of an $n \times n$ matrix, which is just a scalar function of t. Since the trace of A is a scalar, $e^{t\,\mathrm{Tr}\,(A)}$ is also a scalar function of the variable t. Now,

$$\begin{aligned} e^{tA} &= \sum_{k=0}^{\infty} \frac{(tA)^k}{k!} \\ &= \sum_{k=0}^{\infty} t^k \frac{(P^{-1}DP)^k}{k!} \\ &= P^{-1}\Big[\sum_{k=0}^{\infty} t^k \frac{D^k}{k!}\Big]P\,. \end{aligned} \tag{29}$$

Wait! Does that makes sense to pull P^{-1} and P to the outsides? Well, $(P^{-1}DP)^k = P^{-1}D^kP$, so it does. (It's easy to prove.)

Now we take the determinant of both sides.

$$
\begin{aligned}
\det e^{tA} &= \det\Big(P^{-1}\big[\sum_{k=0}^{\infty} t^k \frac{D^k}{k!}\big]P\Big) \\
&= \det(P^{-1})\det\big[\sum_{k=0}^{\infty} t^k \frac{D^k}{k!}\big]\det(P) \\
&= \det\big[\sum_{k=0}^{\infty} t^k \frac{D^k}{k!}\big] \\
&= \det\big[\,\mathrm{diag}\Big(\sum_{k=0}^{\infty} t^k \frac{d_{11}^k}{k!}, \sum_{k=0}^{\infty} t^k \frac{d_{22}^k}{k!}, \ldots, \sum_{k=0}^{\infty} t^k \frac{d_{nn}^k}{k!}\Big)\big] \\
&= \det\big[\mathrm{diag}\big(e^{td_{11}}, e^{td_{22}}, \ldots, e^{td_{nn}}\big)\big] \\
&= e^{td_{11}} e^{td_{22}} \cdots e^{td_{nn}} = e^{t(d_{11}+d_{22}+\cdots+d_{nn})} \\
&= e^{t\,\mathrm{Tr}\,(D)} \\
&= e^{t\,\mathrm{Tr}\,(A)}\,. \qquad (30)
\end{aligned}
$$

And this is all I have for traces in this paper, though I expect to have a follow-up paper soon about the applications of the trace function as it is used in the Dirac theory.