

Appendix D

Matrix calculus

From too much study, and from extreme passion, cometh madnesse.

– Isaac Newton [179, §5]

D.1 Gradient, Directional derivative, Taylor series

D.1.1 Gradients

Gradient of a differentiable real function $f(x) : \mathbb{R}^K \rightarrow \mathbb{R}$ with respect to its vector argument is defined uniquely in terms of partial derivatives

$$\nabla f(x) \triangleq \begin{bmatrix} \frac{\partial f(x)}{\partial x_1} \\ \frac{\partial f(x)}{\partial x_2} \\ \vdots \\ \frac{\partial f(x)}{\partial x_K} \end{bmatrix} \in \mathbb{R}^K \quad (1955)$$

while the second-order gradient of the twice differentiable real function with respect to its vector argument is traditionally called the *Hessian*;

$$\nabla^2 f(x) \triangleq \begin{bmatrix} \frac{\partial^2 f(x)}{\partial x_1^2} & \frac{\partial^2 f(x)}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_1 \partial x_K} \\ \frac{\partial^2 f(x)}{\partial x_2 \partial x_1} & \frac{\partial^2 f(x)}{\partial x_2^2} & \cdots & \frac{\partial^2 f(x)}{\partial x_2 \partial x_K} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f(x)}{\partial x_K \partial x_1} & \frac{\partial^2 f(x)}{\partial x_K \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_K^2} \end{bmatrix} \in \mathbb{S}^K \quad (1956)$$

The gradient of vector-valued function $v(x) : \mathbb{R} \rightarrow \mathbb{R}^N$ on real domain is a row vector

$$\nabla v(x) \triangleq \begin{bmatrix} \frac{\partial v_1(x)}{\partial x} & \frac{\partial v_2(x)}{\partial x} & \cdots & \frac{\partial v_N(x)}{\partial x} \end{bmatrix} \in \mathbb{R}^N \quad (1957)$$

while the second-order gradient is

$$\nabla^2 v(x) \triangleq \begin{bmatrix} \frac{\partial^2 v_1(x)}{\partial x^2} & \frac{\partial^2 v_2(x)}{\partial x^2} & \cdots & \frac{\partial^2 v_N(x)}{\partial x^2} \end{bmatrix} \in \mathbb{R}^N \quad (1958)$$

Gradient of vector-valued function $h(x) : \mathbb{R}^K \rightarrow \mathbb{R}^N$ on vector domain is

$$\begin{aligned} \nabla h(x) &\triangleq \begin{bmatrix} \frac{\partial h_1(x)}{\partial x_1} & \frac{\partial h_2(x)}{\partial x_1} & \cdots & \frac{\partial h_N(x)}{\partial x_1} \\ \frac{\partial h_1(x)}{\partial x_2} & \frac{\partial h_2(x)}{\partial x_2} & \cdots & \frac{\partial h_N(x)}{\partial x_2} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial h_1(x)}{\partial x_K} & \frac{\partial h_2(x)}{\partial x_K} & \cdots & \frac{\partial h_N(x)}{\partial x_K} \end{bmatrix} \\ &= [\nabla h_1(x) \quad \nabla h_2(x) \quad \cdots \quad \nabla h_N(x)] \in \mathbb{R}^{K \times N} \end{aligned} \quad (1959)$$

while the second-order gradient has a three-dimensional written representation dubbed *cubix*; [D.1](#)

$$\begin{aligned} \nabla^2 h(x) &\triangleq \begin{bmatrix} \nabla \frac{\partial h_1(x)}{\partial x_1} & \nabla \frac{\partial h_2(x)}{\partial x_1} & \cdots & \nabla \frac{\partial h_N(x)}{\partial x_1} \\ \nabla \frac{\partial h_1(x)}{\partial x_2} & \nabla \frac{\partial h_2(x)}{\partial x_2} & \cdots & \nabla \frac{\partial h_N(x)}{\partial x_2} \\ \vdots & \vdots & \ddots & \vdots \\ \nabla \frac{\partial h_1(x)}{\partial x_K} & \nabla \frac{\partial h_2(x)}{\partial x_K} & \cdots & \nabla \frac{\partial h_N(x)}{\partial x_K} \end{bmatrix} \\ &= [\nabla^2 h_1(x) \quad \nabla^2 h_2(x) \quad \cdots \quad \nabla^2 h_N(x)] \in \mathbb{R}^{K \times N \times K} \end{aligned} \quad (1960)$$

where the gradient of each real entry is with respect to vector x as in [\(1955\)](#).

The gradient of real function $g(X) : \mathbb{R}^{K \times L} \rightarrow \mathbb{R}$ on matrix domain is

$$\begin{aligned} \nabla g(X) &\triangleq \begin{bmatrix} \frac{\partial g(X)}{\partial X_{11}} & \frac{\partial g(X)}{\partial X_{12}} & \cdots & \frac{\partial g(X)}{\partial X_{1L}} \\ \frac{\partial g(X)}{\partial X_{21}} & \frac{\partial g(X)}{\partial X_{22}} & \cdots & \frac{\partial g(X)}{\partial X_{2L}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial g(X)}{\partial X_{K1}} & \frac{\partial g(X)}{\partial X_{K2}} & \cdots & \frac{\partial g(X)}{\partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K \times L} \\ &= \begin{bmatrix} \nabla_{X(:,1)} g(X) \\ \nabla_{X(:,2)} g(X) \\ \vdots \\ \nabla_{X(:,L)} g(X) \end{bmatrix} \in \mathbb{R}^{K \times 1 \times L} \end{aligned} \quad (1961)$$

where gradient $\nabla_{X(:,i)}$ is with respect to the i^{th} column of X . The strange appearance of [\(1961\)](#) in $\mathbb{R}^{K \times 1 \times L}$ is meant to suggest a third dimension perpendicular to the page (not a diagonal matrix). The second-order gradient has representation

D.1 The word *matrix* comes from the Latin for *womb*; related to the prefix *matri-* derived from *mater* meaning *mother*.

$$\begin{aligned}
\nabla^2 g(X) &\triangleq \begin{bmatrix} \nabla \frac{\partial g(X)}{\partial X_{11}} & \nabla \frac{\partial g(X)}{\partial X_{12}} & \cdots & \nabla \frac{\partial g(X)}{\partial X_{1L}} \\ \nabla \frac{\partial g(X)}{\partial X_{21}} & \nabla \frac{\partial g(X)}{\partial X_{22}} & \cdots & \nabla \frac{\partial g(X)}{\partial X_{2L}} \\ \vdots & \vdots & \ddots & \vdots \\ \nabla \frac{\partial g(X)}{\partial X_{K1}} & \nabla \frac{\partial g(X)}{\partial X_{K2}} & \cdots & \nabla \frac{\partial g(X)}{\partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K \times L \times K \times L} \\
&= \begin{bmatrix} \nabla \nabla_{X(:,1)} g(X) \\ \nabla \nabla_{X(:,2)} g(X) \\ \vdots \\ \nabla \nabla_{X(:,L)} g(X) \end{bmatrix} \in \mathbb{R}^{K \times 1 \times L \times K \times L}
\end{aligned} \tag{1962}$$

where the gradient ∇ is with respect to matrix X .

Gradient of vector-valued function $g(X) : \mathbb{R}^{K \times L} \rightarrow \mathbb{R}^N$ on matrix domain is a cubix

$$\begin{aligned}
\nabla g(X) &\triangleq \begin{bmatrix} \nabla_{X(:,1)} g_1(X) & \nabla_{X(:,1)} g_2(X) & \cdots & \nabla_{X(:,1)} g_N(X) \\ \nabla_{X(:,2)} g_1(X) & \nabla_{X(:,2)} g_2(X) & \cdots & \nabla_{X(:,2)} g_N(X) \\ \vdots & \vdots & \ddots & \vdots \\ \nabla_{X(:,L)} g_1(X) & \nabla_{X(:,L)} g_2(X) & \cdots & \nabla_{X(:,L)} g_N(X) \end{bmatrix} \\
&= [\nabla g_1(X) \quad \nabla g_2(X) \quad \cdots \quad \nabla g_N(X)] \in \mathbb{R}^{K \times N \times L}
\end{aligned} \tag{1963}$$

while the second-order gradient has a five-dimensional representation;

$$\begin{aligned}
\nabla^2 g(X) &\triangleq \begin{bmatrix} \nabla \nabla_{X(:,1)} g_1(X) & \nabla \nabla_{X(:,1)} g_2(X) & \cdots & \nabla \nabla_{X(:,1)} g_N(X) \\ \nabla \nabla_{X(:,2)} g_1(X) & \nabla \nabla_{X(:,2)} g_2(X) & \cdots & \nabla \nabla_{X(:,2)} g_N(X) \\ \vdots & \vdots & \ddots & \vdots \\ \nabla \nabla_{X(:,L)} g_1(X) & \nabla \nabla_{X(:,L)} g_2(X) & \cdots & \nabla \nabla_{X(:,L)} g_N(X) \end{bmatrix} \\
&= [\nabla^2 g_1(X) \quad \nabla^2 g_2(X) \quad \cdots \quad \nabla^2 g_N(X)] \in \mathbb{R}^{K \times N \times L \times K \times L}
\end{aligned} \tag{1964}$$

The gradient of matrix-valued function $g(X) : \mathbb{R}^{K \times L} \rightarrow \mathbb{R}^{M \times N}$ on matrix domain has a four-dimensional representation called *quartix* (*fourth-order tensor*)

$$\nabla g(X) \triangleq \begin{bmatrix} \nabla g_{11}(X) & \nabla g_{12}(X) & \cdots & \nabla g_{1N}(X) \\ \nabla g_{21}(X) & \nabla g_{22}(X) & \cdots & \nabla g_{2N}(X) \\ \vdots & \vdots & \ddots & \vdots \\ \nabla g_{M1}(X) & \nabla g_{M2}(X) & \cdots & \nabla g_{MN}(X) \end{bmatrix} \in \mathbb{R}^{M \times N \times K \times L} \tag{1965}$$

while the second-order gradient has a six-dimensional representation

$$\nabla^2 g(X) \triangleq \begin{bmatrix} \nabla^2 g_{11}(X) & \nabla^2 g_{12}(X) & \cdots & \nabla^2 g_{1N}(X) \\ \nabla^2 g_{21}(X) & \nabla^2 g_{22}(X) & \cdots & \nabla^2 g_{2N}(X) \\ \vdots & \vdots & \ddots & \vdots \\ \nabla^2 g_{M1}(X) & \nabla^2 g_{M2}(X) & \cdots & \nabla^2 g_{MN}(X) \end{bmatrix} \in \mathbb{R}^{M \times N \times K \times L \times K \times L} \tag{1966}$$

and so on.

D.1.2 Product rules for matrix-functions

Given dimensionally compatible matrix-valued functions of matrix variable $f(X)$ and $g(X)$

$$\nabla_X (f(X)^T g(X)) = \nabla_X(f) g + \nabla_X(g) f \quad (1967)$$

while [57, §8.3] [358]

$$\nabla_X \operatorname{tr}(f(X)^T g(X)) = \nabla_X \left(\operatorname{tr}(f(X)^T g(X)) + \operatorname{tr}(g(X) f(X)^T) \right) \Big|_{Z \leftarrow X} \quad (1968)$$

These expressions implicitly apply as well to scalar-, vector-, or matrix-valued functions of scalar, vector, or matrix arguments.

D.1.2.0.1 Example. Cubix.

Suppose $f(X) : \mathbb{R}^{2 \times 2} \rightarrow \mathbb{R}^2 = X^T a$ and $g(X) : \mathbb{R}^{2 \times 2} \rightarrow \mathbb{R}^2 = X b$. We wish to find

$$\nabla_X (f(X)^T g(X)) = \nabla_X a^T X^2 b \quad (1969)$$

using the product rule. Formula (1967) calls for

$$\nabla_X a^T X^2 b = \nabla_X (X^T a) X b + \nabla_X (X b) X^T a \quad (1970)$$

Consider the first of the two terms:

$$\begin{aligned} \nabla_X(f) g &= \nabla_X (X^T a) X b \\ &= \begin{bmatrix} \nabla(X^T a)_1 & \nabla(X^T a)_2 \end{bmatrix} X b \end{aligned} \quad (1971)$$

The gradient of $X^T a$ forms a cubix in $\mathbb{R}^{2 \times 2 \times 2}$; **a.k.a.**, *third-order tensor*.

$$\nabla_X (X^T a) X b = \left[\begin{array}{ccc} \frac{\partial(X^T a)_1}{\partial X_{11}} & \cdots & \frac{\partial(X^T a)_2}{\partial X_{11}} \\ & \searrow & \searrow \\ & \frac{\partial(X^T a)_1}{\partial X_{12}} & \cdots & \frac{\partial(X^T a)_2}{\partial X_{12}} \\ & & & \searrow & \searrow \\ \frac{\partial(X^T a)_1}{\partial X_{21}} & \cdots & \frac{\partial(X^T a)_2}{\partial X_{21}} & & \\ & & & \searrow & \searrow \\ & \frac{\partial(X^T a)_1}{\partial X_{22}} & \cdots & \frac{\partial(X^T a)_2}{\partial X_{22}} \end{array} \right] \begin{bmatrix} (Xb)_1 \\ (Xb)_2 \end{bmatrix} \in \mathbb{R}^{2 \times 1 \times 2} \quad (1972)$$

Because gradient of the product (1969) requires total change with respect to change in each entry of matrix X , the Xb vector must make an inner product with each vector in that second dimension of the cubix indicated by dotted line segments;

$$\begin{aligned} \nabla_X (X^T a) X b &= \begin{bmatrix} a_1 & 0 \\ & 0 & a_1 \\ a_2 & 0 \\ & 0 & a_2 \end{bmatrix} \begin{bmatrix} b_1 X_{11} + b_2 X_{12} \\ b_1 X_{21} + b_2 X_{22} \end{bmatrix} \in \mathbb{R}^{2 \times 1 \times 2} \\ &= \begin{bmatrix} a_1(b_1 X_{11} + b_2 X_{12}) & a_1(b_1 X_{21} + b_2 X_{22}) \\ a_2(b_1 X_{11} + b_2 X_{12}) & a_2(b_1 X_{21} + b_2 X_{22}) \end{bmatrix} \in \mathbb{R}^{2 \times 2} \\ &= ab^T X^T \end{aligned} \quad (1973)$$

where the cubix appears as a complete $2 \times 2 \times 2$ matrix. In like manner for the second term $\nabla_X(g) f$

$$\begin{aligned}\nabla_X(Xb) X^T a &= \begin{bmatrix} b_1 & 0 & 0 \\ 0 & b_2 & 0 \\ 0 & 0 & b_1 \\ 0 & 0 & b_2 \end{bmatrix} \begin{bmatrix} X_{11}a_1 + X_{21}a_2 \\ X_{12}a_1 + X_{22}a_2 \end{bmatrix} \in \mathbb{R}^{2 \times 1 \times 2} \\ &= X^T ab^T \in \mathbb{R}^{2 \times 2}\end{aligned}\quad (1974)$$

The solution

$$\nabla_X a^T X^2 b = ab^T X^T + X^T ab^T \quad (1975)$$

can be found from Table D.2.1 or verified using (1968). \square

D.1.2.1 Kronecker product

A partial remedy for venturing into *hyperdimensional* matrix representations, such as the cubix or quartix, is to first vectorize matrices as in (39). This device gives rise to the Kronecker product of matrices \otimes ; a.k.a, *tensor product* (`kron()` in Matlab). Although its definition sees reversal in the literature, [369, §2.1] Kronecker product is not commutative ($B \otimes A \neq A \otimes B$). We adopt the definition: for $A \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{p \times q}$

$$B \otimes A \triangleq \begin{bmatrix} B_{11}A & B_{12}A & \cdots & B_{1q}A \\ B_{21}A & B_{22}A & \cdots & B_{2q}A \\ \vdots & \vdots & \ddots & \vdots \\ B_{p1}A & B_{p2}A & \cdots & B_{pq}A \end{bmatrix} \in \mathbb{R}^{pm \times qn} \quad (1976)$$

for which $A \otimes 1 = 1 \otimes A = A$ (real unity acts like Identity).

One advantage to vectorization is existence of the traditional two-dimensional matrix representation (*second-order tensor*) for the second-order gradient of a real function with respect to a vectorized matrix. From §A.1.1 no.36 (§D.2.1) for square $A, B \in \mathbb{R}^{n \times n}$, for example [194, §5.2] [14, §3]

$$\nabla_{\text{vec } X}^2 \text{tr}(AXBX^T) = \nabla_{\text{vec } X}^2 \text{vec}(X)^T (B^T \otimes A) \text{vec } X = B \otimes A^T + B^T \otimes A \in \mathbb{R}^{n^2 \times n^2} \quad (1977)$$

To disadvantage is a large new but known set of algebraic rules (§A.1.1) and the fact that its mere use does not generally guarantee two-dimensional matrix representation of gradients.

Another application of the Kronecker product is to reverse order of appearance in a matrix product: Suppose we wish to weight the columns of a matrix $S \in \mathbb{R}^{M \times N}$, for example, by respective entries w_i from the main diagonal in

$$W \triangleq \begin{bmatrix} w_1 & & \mathbf{0} \\ & \ddots & \\ \mathbf{0} & & w_N \end{bmatrix} \in \mathbb{S}^N \quad (1978)$$

A conventional means for accomplishing column weighting is to multiply S by diagonal matrix W on the right side:

$$SW = S \begin{bmatrix} w_1 & & \mathbf{0} \\ & \ddots & \\ \mathbf{0} & & w_N \end{bmatrix} = [S(:, 1)w_1 \quad \cdots \quad S(:, N)w_N] \in \mathbb{R}^{M \times N} \quad (1979)$$

To reverse product order such that diagonal matrix W instead appears to the left of S : for $I \in \mathbb{S}^M$ (Law)

$$SW = (\delta(W)^T \otimes I) \begin{bmatrix} S(:, 1) & 0 & & \mathbf{0} \\ 0 & S(:, 2) & \ddots & \\ & \ddots & \ddots & 0 \\ \mathbf{0} & & 0 & S(:, N) \end{bmatrix} \in \mathbb{R}^{M \times N} \quad (1980)$$

To instead weight the rows of S via diagonal matrix $W \in \mathbb{S}^M$, for $I \in \mathbb{S}^N$

$$WS = \begin{bmatrix} S(1, :) & 0 & & \mathbf{0} \\ 0 & S(2, :) & \ddots & \\ & \ddots & \ddots & 0 \\ \mathbf{0} & & 0 & S(M, :) \end{bmatrix} (\delta(W) \otimes I) \in \mathbb{R}^{M \times N} \quad (1981)$$

D.1.2.2 Hadamard product

For any matrices of like size, $S, Y \in \mathbb{R}^{M \times N}$, Hadamard's product \circ denotes simple multiplication of corresponding entries (\cdot in Matlab). It is possible to convert Hadamard product into a standard product of matrices:

$$S \circ Y = [\delta(Y(:, 1)) \cdots \delta(Y(:, N))] \begin{bmatrix} S(:, 1) & 0 & & \mathbf{0} \\ 0 & S(:, 2) & \ddots & \\ & \ddots & \ddots & 0 \\ \mathbf{0} & & 0 & S(:, N) \end{bmatrix} \in \mathbb{R}^{M \times N} \quad (1982)$$

In the special case that $S = s$ and $Y = y$ are vectors in \mathbb{R}^M

$$s \circ y = \delta(s)y \quad (1983)$$

$$\begin{aligned} s^T \otimes y &= ys^T \\ s \otimes y^T &= sy^T \end{aligned} \quad (1984)$$

D.1.3 Chain rules for composite matrix-functions

Given dimensionally compatible matrix-valued functions of matrix variable $f(X)$ and $g(X)$ [393, §15.7]

$$\nabla_X g(f(X)^T) = \nabla_X f^T \nabla_f g \quad (1985)$$

$$\nabla_X^2 g(f(X)^T) = \nabla_X (\nabla_X f^T \nabla_f g) = \nabla_X^2 f \nabla_f g + \nabla_X f^T \nabla_f^2 g \nabla_X f \quad (1986)$$

D.1.3.1 Two arguments

$$\nabla_X g(f(X)^T, h(X)^T) = \nabla_X f^T \nabla_f g + \nabla_X h^T \nabla_h g \quad (1987)$$

D.1.3.1.1 Example. *Chain rule for two arguments.* [44, §1.1]

$$g(f(x)^T, h(x)^T) = (f(x) + h(x))^T A (f(x) + h(x)) \quad (1988)$$

$$f(x) = \begin{bmatrix} x_1 \\ \varepsilon x_2 \end{bmatrix}, \quad h(x) = \begin{bmatrix} \varepsilon x_1 \\ x_2 \end{bmatrix} \quad (1989)$$

$$\nabla_x g(f(x)^T, h(x)^T) = \begin{bmatrix} 1 & 0 \\ 0 & \varepsilon \end{bmatrix} (A + A^T)(f + h) + \begin{bmatrix} \varepsilon & 0 \\ 0 & 1 \end{bmatrix} (A + A^T)(f + h) \quad (1990)$$

$$\nabla_x g(f(x)^T, h(x)^T) = \begin{bmatrix} 1 + \varepsilon & 0 \\ 0 & 1 + \varepsilon \end{bmatrix} (A + A^T) \left(\begin{bmatrix} x_1 \\ \varepsilon x_2 \end{bmatrix} + \begin{bmatrix} \varepsilon x_1 \\ x_2 \end{bmatrix} \right) \quad (1991)$$

$$\lim_{\varepsilon \rightarrow 0} \nabla_x g(f(x)^T, h(x)^T) = (A + A^T)x \quad (1992)$$

from Table D.2.1. □

These foregoing formulae remain correct when gradient produces hyperdimensional representation:

D.1.4 First directional derivative

Assume that a differentiable function $g(X) : \mathbb{R}^{K \times L} \rightarrow \mathbb{R}^{M \times N}$ has continuous first- and second-order gradients ∇g and $\nabla^2 g$ over $\text{dom } g$ which is an open set. We seek simple expressions for the first and second directional derivatives in direction $Y \in \mathbb{R}^{K \times L}$: respectively, $\vec{D}g \in \mathbb{R}^{M \times N}$ and $\vec{D}g^2 \in \mathbb{R}^{M \times N}$.

Assuming that the limit exists, we may state the partial derivative of the mn^{th} entry of g with respect to kl^{th} entry of X ;

$$\frac{\partial g_{mn}(X)}{\partial X_{kl}} = \lim_{\Delta t \rightarrow 0} \frac{g_{mn}(X + \Delta t e_k e_l^T) - g_{mn}(X)}{\Delta t} \in \mathbb{R} \quad (1993)$$

where e_k is the k^{th} standard basis vector in \mathbb{R}^K while e_l is the l^{th} standard basis vector in \mathbb{R}^L . Total number of partial derivatives equals $KLMN$ while the gradient is defined in their terms; mn^{th} entry of the gradient is

$$\nabla g_{mn}(X) = \begin{bmatrix} \frac{\partial g_{mn}(X)}{\partial X_{11}} & \frac{\partial g_{mn}(X)}{\partial X_{12}} & \cdots & \frac{\partial g_{mn}(X)}{\partial X_{1L}} \\ \frac{\partial g_{mn}(X)}{\partial X_{21}} & \frac{\partial g_{mn}(X)}{\partial X_{22}} & \cdots & \frac{\partial g_{mn}(X)}{\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \frac{\partial g_{mn}(X)}{\partial X_{K1}} & \frac{\partial g_{mn}(X)}{\partial X_{K2}} & \cdots & \frac{\partial g_{mn}(X)}{\partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K \times L} \quad (1994)$$

while the gradient is a quartix

$$\nabla g(X) = \begin{bmatrix} \nabla g_{11}(X) & \nabla g_{12}(X) & \cdots & \nabla g_{1N}(X) \\ \nabla g_{21}(X) & \nabla g_{22}(X) & \cdots & \nabla g_{2N}(X) \\ \vdots & \vdots & & \vdots \\ \nabla g_{M1}(X) & \nabla g_{M2}(X) & \cdots & \nabla g_{MN}(X) \end{bmatrix} \in \mathbb{R}^{M \times N \times K \times L} \quad (1995)$$

By simply rotating our perspective of a four-dimensional representation of gradient matrix, we find one of three useful transpositions of this quartix (connoted T_1):

$$\nabla g(X)^{T_1} = \begin{bmatrix} \frac{\partial g(X)}{\partial X_{11}} & \frac{\partial g(X)}{\partial X_{12}} & \cdots & \frac{\partial g(X)}{\partial X_{1L}} \\ \frac{\partial g(X)}{\partial X_{21}} & \frac{\partial g(X)}{\partial X_{22}} & \cdots & \frac{\partial g(X)}{\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \frac{\partial g(X)}{\partial X_{K1}} & \frac{\partial g(X)}{\partial X_{K2}} & \cdots & \frac{\partial g(X)}{\partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K \times L \times M \times N} \quad (1996)$$

When a limit for $\Delta t \in \mathbb{R}$ exists, it is easy to show by substitution of variables in (1993)

$$\frac{\partial g_{mn}(X)}{\partial X_{kl}} Y_{kl} = \lim_{\Delta t \rightarrow 0} \frac{g_{mn}(X + \Delta t Y_{kl} e_k e_l^T) - g_{mn}(X)}{\Delta t} \in \mathbb{R} \quad (1997)$$

which may be interpreted as the change in g_{mn} at X when the change in X_{kl} is equal to Y_{kl} the kl^{th} entry of any $Y \in \mathbb{R}^{K \times L}$. Because the total change in $g_{mn}(X)$ due to Y is the sum of change with respect to each and every X_{kl} , the mn^{th} entry of the directional derivative is the corresponding total differential [393, §15.8]

$$dg_{mn}(X)|_{dX \rightarrow Y} = \sum_{k,l} \frac{\partial g_{mn}(X)}{\partial X_{kl}} Y_{kl} = \text{tr}(\nabla g_{mn}(X)^T Y) \quad (1998)$$

$$= \sum_{k,l} \lim_{\Delta t \rightarrow 0} \frac{g_{mn}(X + \Delta t Y_{kl} e_k e_l^T) - g_{mn}(X)}{\Delta t} \quad (1999)$$

$$= \lim_{\Delta t \rightarrow 0} \frac{g_{mn}(X + \Delta t Y) - g_{mn}(X)}{\Delta t} \quad (2000)$$

$$= \left. \frac{d}{dt} \right|_{t=0} g_{mn}(X + t Y) \quad (2001)$$

where $t \in \mathbb{R}$. Assuming finite Y , equation (2000) is called the *Gâteaux differential* [43, App.A.5] [230, §D.2.1] [405, §5.28] whose existence is implied by existence of the *Fréchet differential* (the sum in (1998)). [285, §7.2] Each may be understood as the change in g_{mn} at X when the change in X is equal in magnitude and direction to Y .^{D.2} Hence the directional derivative,

$$\begin{aligned} \overset{\rightarrow}{dg}(X) &\triangleq \left[\begin{array}{cccc} dg_{11}(X) & dg_{12}(X) & \cdots & dg_{1N}(X) \\ dg_{21}(X) & dg_{22}(X) & \cdots & dg_{2N}(X) \\ \vdots & \vdots & & \vdots \\ dg_{M1}(X) & dg_{M2}(X) & \cdots & dg_{MN}(X) \end{array} \right] \bigg|_{dX \rightarrow Y} \in \mathbb{R}^{M \times N} \\ &= \left[\begin{array}{cccc} \text{tr}(\nabla g_{11}(X)^T Y) & \text{tr}(\nabla g_{12}(X)^T Y) & \cdots & \text{tr}(\nabla g_{1N}(X)^T Y) \\ \text{tr}(\nabla g_{21}(X)^T Y) & \text{tr}(\nabla g_{22}(X)^T Y) & \cdots & \text{tr}(\nabla g_{2N}(X)^T Y) \\ \vdots & \vdots & & \vdots \\ \text{tr}(\nabla g_{M1}(X)^T Y) & \text{tr}(\nabla g_{M2}(X)^T Y) & \cdots & \text{tr}(\nabla g_{MN}(X)^T Y) \end{array} \right] \quad (2002) \\ &= \left[\begin{array}{cccc} \sum_{k,l} \frac{\partial g_{11}(X)}{\partial X_{kl}} Y_{kl} & \sum_{k,l} \frac{\partial g_{12}(X)}{\partial X_{kl}} Y_{kl} & \cdots & \sum_{k,l} \frac{\partial g_{1N}(X)}{\partial X_{kl}} Y_{kl} \\ \sum_{k,l} \frac{\partial g_{21}(X)}{\partial X_{kl}} Y_{kl} & \sum_{k,l} \frac{\partial g_{22}(X)}{\partial X_{kl}} Y_{kl} & \cdots & \sum_{k,l} \frac{\partial g_{2N}(X)}{\partial X_{kl}} Y_{kl} \\ \vdots & \vdots & & \vdots \\ \sum_{k,l} \frac{\partial g_{M1}(X)}{\partial X_{kl}} Y_{kl} & \sum_{k,l} \frac{\partial g_{M2}(X)}{\partial X_{kl}} Y_{kl} & \cdots & \sum_{k,l} \frac{\partial g_{MN}(X)}{\partial X_{kl}} Y_{kl} \end{array} \right] \end{aligned}$$

from which it follows

$$\overset{\rightarrow}{dg}(X) = \sum_{k,l} \frac{\partial g(X)}{\partial X_{kl}} Y_{kl} \quad (2003)$$

Yet for all $X \in \text{dom } g$, any $Y \in \mathbb{R}^{K \times L}$, and some open interval of $t \in \mathbb{R}$

$$g(X + t Y) = g(X) + t \overset{\rightarrow}{dg}(X) + O(t^2) \quad (2004)$$

which is the first-order multidimensional Taylor series expansion about X . [393, §18.4] [177, §2.3.4] Differentiation with respect to t and subsequent t -zeroing isolates the second term of expansion. Thus differentiating and zeroing $g(X + t Y)$ in t is an operation equivalent to individually differentiating and zeroing every entry $g_{mn}(X + t Y)$ as in (2001). So the directional derivative of $g(X) : \mathbb{R}^{K \times L} \rightarrow \mathbb{R}^{M \times N}$ in any direction $Y \in \mathbb{R}^{K \times L}$ evaluated at $X \in \text{dom } g$ becomes

$$\overset{\rightarrow}{dg}(X) = \left. \frac{d}{dt} \right|_{t=0} g(X + t Y) \in \mathbb{R}^{M \times N} \quad (2005)$$

^{D.2}Although Y is a matrix, we may regard it as a vector in \mathbb{R}^{KL} .

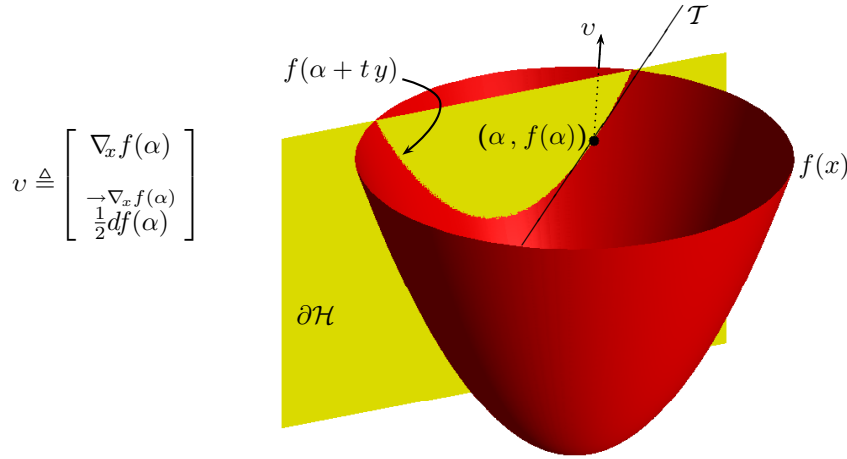


Figure 189: Strictly convex quadratic bowl in $\mathbb{R}^2 \times \mathbb{R}$; $f(x) = x^T x : \mathbb{R}^2 \rightarrow \mathbb{R}$ versus x on some open disc in \mathbb{R}^2 . Plane slice $\partial\mathcal{H}$ is perpendicular to function domain. Slice intersection with domain connotes bidirectional vector y . Slope of tangent line \mathcal{T} at point $(\alpha, f(\alpha))$ is value of directional derivative $\nabla_x f(\alpha)^T y$ (2030) at α in slice direction y . Negative gradient $-\nabla_x f(x) \in \mathbb{R}^2$ is direction of *steepest descent*. [393, §15.6] [177] When vector $v \in \mathbb{R}^3$ entry v_3 is half directional derivative in gradient direction at α and when $\begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = \nabla_x f(\alpha)$, then $-v$ points directly toward bowl bottom.

[315, §2.1, §5.4.5] [36, §6.3.1] which is simplest. In case of a real function $g(X) : \mathbb{R}^{K \times L} \rightarrow \mathbb{R}$

$$\overset{\rightarrow Y}{dg}(X) = \text{tr}(\nabla g(X)^T Y) \quad (2027)$$

In case $g(X) : \mathbb{R}^K \rightarrow \mathbb{R}$

$$\overset{\rightarrow Y}{dg}(X) = \nabla g(X)^T Y \quad (2030)$$

Unlike gradient, directional derivative does not expand dimension; directional derivative (2005) retains the dimensions of g . The derivative with respect to t makes the directional derivative resemble ordinary calculus (§D.2); *e.g.*, when $g(X)$ is linear, $\overset{\rightarrow Y}{dg}(X) = g(Y)$. [285, §7.2]

D.1.4.1 Interpretation of directional derivative

In the case of any differentiable real function $g(X) : \mathbb{R}^{K \times L} \rightarrow \mathbb{R}$, the directional derivative of $g(X)$ at X in any direction Y yields the slope of g along the line $\{X + tY \mid t \in \mathbb{R}\}$ through its domain evaluated at $t = 0$. For higher-dimensional functions, by (2002), this slope interpretation can be applied to each entry of the directional derivative.

Figure 189, for example, shows a plane slice of a real convex bowl-shaped function $f(x)$ along a line $\{\alpha + ty \mid t \in \mathbb{R}\}$ through its domain. The slice reveals a one-dimensional real function of t ; $f(\alpha + ty)$. The directional derivative at $x = \alpha$ in direction y is the slope of $f(\alpha + ty)$ with respect to t at $t = 0$. In the case of a real function having vector argument $h(X) : \mathbb{R}^K \rightarrow \mathbb{R}$, its directional derivative in the normalized direction of its gradient is the gradient magnitude. (2030) For a real function of real variable, the directional derivative evaluated at any point in the function domain is just the slope of that function there scaled by the real direction. (*confer* §3.6)

Directional derivative generalizes our one-dimensional notion of derivative to a multidimensional domain. When direction Y coincides with a member of the standard Cartesian basis $e_k e_l^T$ (63), then a single partial derivative $\partial g(X)/\partial X_{kl}$ is obtained from directional derivative (2003); such is each entry of gradient $\nabla g(X)$ in equalities (2027) and (2030), for example.

D.1.4.1.1 Theorem. *Directional derivative optimality condition.* [285, §7.4] Suppose $f(X) : \mathbb{R}^{K \times L} \rightarrow \mathbb{R}$ is minimized on convex set $\mathcal{C} \subseteq \mathbb{R}^{K \times L}$ by X^* , and the directional derivative of f exists there. Then for all $X \in \mathcal{C}$

$$\begin{matrix} \rightarrow X - X^* \\ df(X) \end{matrix} \geq 0 \quad (2006)$$

◇

D.1.4.1.2 Example. *Simple bowl.*
Bowl function (Figure 189)

$$f(x) : \mathbb{R}^K \rightarrow \mathbb{R} \triangleq (x - a)^T(x - a) - b \quad (2007)$$

has function offset $-b \in \mathbb{R}$, axis of revolution at $x = a$, and positive definite Hessian (1956) everywhere in its domain (an open *hyperdisc* in \mathbb{R}^K); *id est*, strictly convex quadratic $f(x)$ has unique global minimum equal to $-b$ at $x = a$. A vector $-v$ based anywhere in $\text{dom } f \times \mathbb{R}$ pointing toward the unique bowl-bottom is specified:

$$v \propto \begin{bmatrix} x - a \\ f(x) + b \end{bmatrix} \in \mathbb{R}^K \times \mathbb{R} \quad (2008)$$

Such a vector is

$$v = \begin{bmatrix} \nabla_x f(x) \\ \frac{1}{2} df(x) \end{bmatrix} \quad (2009)$$

since the gradient is

$$\nabla_x f(x) = 2(x - a) \quad (2010)$$

and the directional derivative in direction of the gradient is (2030)

$$\begin{matrix} \rightarrow \nabla_x f(x) \\ df(x) \end{matrix} = \nabla_x f(x)^T \nabla_x f(x) = 4(x - a)^T(x - a) = 4(f(x) + b) \quad (2011)$$

□

D.1.5 Second directional derivative

By similar argument, it so happens: the second directional derivative is equally simple. Given $g(X) : \mathbb{R}^{K \times L} \rightarrow \mathbb{R}^{M \times N}$ on open domain,

$$\nabla \frac{\partial g_{mn}(X)}{\partial X_{kl}} = \frac{\partial \nabla g_{mn}(X)}{\partial X_{kl}} = \begin{bmatrix} \frac{\partial^2 g_{mn}(X)}{\partial X_{kl} \partial X_{11}} & \frac{\partial^2 g_{mn}(X)}{\partial X_{kl} \partial X_{12}} & \cdots & \frac{\partial^2 g_{mn}(X)}{\partial X_{kl} \partial X_{1L}} \\ \frac{\partial^2 g_{mn}(X)}{\partial X_{kl} \partial X_{21}} & \frac{\partial^2 g_{mn}(X)}{\partial X_{kl} \partial X_{22}} & \cdots & \frac{\partial^2 g_{mn}(X)}{\partial X_{kl} \partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \frac{\partial^2 g_{mn}(X)}{\partial X_{kl} \partial X_{K1}} & \frac{\partial^2 g_{mn}(X)}{\partial X_{kl} \partial X_{K2}} & \cdots & \frac{\partial^2 g_{mn}(X)}{\partial X_{kl} \partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K \times L} \quad (2012)$$

$$\begin{aligned}
\nabla^2 g_{mn}(X) &= \begin{bmatrix} \nabla \frac{\partial g_{mn}(X)}{\partial X_{11}} & \nabla \frac{\partial g_{mn}(X)}{\partial X_{12}} & \cdots & \nabla \frac{\partial g_{mn}(X)}{\partial X_{1L}} \\ \nabla \frac{\partial g_{mn}(X)}{\partial X_{21}} & \nabla \frac{\partial g_{mn}(X)}{\partial X_{22}} & \cdots & \nabla \frac{\partial g_{mn}(X)}{\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \nabla \frac{\partial g_{mn}(X)}{\partial X_{K1}} & \nabla \frac{\partial g_{mn}(X)}{\partial X_{K2}} & \cdots & \nabla \frac{\partial g_{mn}(X)}{\partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K \times L \times K \times L} \\
&= \begin{bmatrix} \frac{\partial \nabla g_{mn}(X)}{\partial X_{11}} & \frac{\partial \nabla g_{mn}(X)}{\partial X_{12}} & \cdots & \frac{\partial \nabla g_{mn}(X)}{\partial X_{1L}} \\ \frac{\partial \nabla g_{mn}(X)}{\partial X_{21}} & \frac{\partial \nabla g_{mn}(X)}{\partial X_{22}} & \cdots & \frac{\partial \nabla g_{mn}(X)}{\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \frac{\partial \nabla g_{mn}(X)}{\partial X_{K1}} & \frac{\partial \nabla g_{mn}(X)}{\partial X_{K2}} & \cdots & \frac{\partial \nabla g_{mn}(X)}{\partial X_{KL}} \end{bmatrix}
\end{aligned} \tag{2013}$$

Rotating our perspective, we get several views of the second-order gradient:

$$\nabla^2 g(X) = \begin{bmatrix} \nabla^2 g_{11}(X) & \nabla^2 g_{12}(X) & \cdots & \nabla^2 g_{1N}(X) \\ \nabla^2 g_{21}(X) & \nabla^2 g_{22}(X) & \cdots & \nabla^2 g_{2N}(X) \\ \vdots & \vdots & & \vdots \\ \nabla^2 g_{M1}(X) & \nabla^2 g_{M2}(X) & \cdots & \nabla^2 g_{MN}(X) \end{bmatrix} \in \mathbb{R}^{M \times N \times K \times L \times K \times L} \tag{2014}$$

$$\nabla^2 g(X)^{T_1} = \begin{bmatrix} \nabla \frac{\partial g(X)}{\partial X_{11}} & \nabla \frac{\partial g(X)}{\partial X_{12}} & \cdots & \nabla \frac{\partial g(X)}{\partial X_{1L}} \\ \nabla \frac{\partial g(X)}{\partial X_{21}} & \nabla \frac{\partial g(X)}{\partial X_{22}} & \cdots & \nabla \frac{\partial g(X)}{\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \nabla \frac{\partial g(X)}{\partial X_{K1}} & \nabla \frac{\partial g(X)}{\partial X_{K2}} & \cdots & \nabla \frac{\partial g(X)}{\partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K \times L \times M \times N \times K \times L} \tag{2015}$$

$$\nabla^2 g(X)^{T_2} = \begin{bmatrix} \frac{\partial \nabla g(X)}{\partial X_{11}} & \frac{\partial \nabla g(X)}{\partial X_{12}} & \cdots & \frac{\partial \nabla g(X)}{\partial X_{1L}} \\ \frac{\partial \nabla g(X)}{\partial X_{21}} & \frac{\partial \nabla g(X)}{\partial X_{22}} & \cdots & \frac{\partial \nabla g(X)}{\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \frac{\partial \nabla g(X)}{\partial X_{K1}} & \frac{\partial \nabla g(X)}{\partial X_{K2}} & \cdots & \frac{\partial \nabla g(X)}{\partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K \times L \times K \times L \times M \times N} \tag{2016}$$

Assuming the limits to exist, we may state the partial derivative of the mn^{th} entry of g with respect to kl^{th} and ij^{th} entries of X ;

$$\begin{aligned}
\frac{\partial^2 g_{mn}(X)}{\partial X_{kl} \partial X_{ij}} &= \frac{\partial}{\partial X_{ij}} \left(\frac{\partial g_{mn}(X)}{\partial X_{kl}} \right) = \lim_{\Delta t \rightarrow 0} \frac{\partial g_{mn}(X + \Delta t e_k e_l^T) - \partial g_{mn}(X)}{\partial X_{ij} \Delta t} \\
&= \lim_{\Delta \tau, \Delta t \rightarrow 0} \frac{(g_{mn}(X + \Delta t e_k e_l^T + \Delta \tau e_i e_j^T) - g_{mn}(X + \Delta t e_k e_l^T)) - (g_{mn}(X + \Delta \tau e_i e_j^T) - g_{mn}(X))}{\Delta \tau \Delta t}
\end{aligned} \tag{2017}$$

Differentiating (1997) and then scaling by Y_{ij}

$$\begin{aligned}
\frac{\partial^2 g_{mn}(X)}{\partial X_{kl} \partial X_{ij}} Y_{kl} Y_{ij} &= \lim_{\Delta t \rightarrow 0} \frac{\partial g_{mn}(X + \Delta t Y_{kl} e_k e_l^T) - \partial g_{mn}(X)}{\partial X_{ij} \Delta t} Y_{ij} \\
&= \lim_{\Delta \tau, \Delta t \rightarrow 0} \frac{(g_{mn}(X + \Delta t Y_{kl} e_k e_l^T + \Delta \tau Y_{ij} e_i e_j^T) - g_{mn}(X + \Delta t Y_{kl} e_k e_l^T)) - (g_{mn}(X + \Delta \tau Y_{ij} e_i e_j^T) - g_{mn}(X))}{\Delta \tau \Delta t}
\end{aligned} \tag{2018}$$

which can be proved by substitution of variables in (2017). The mn^{th} second-order total differential due to any $Y \in \mathbb{R}^{K \times L}$ is

$$d^2g_{mn}(X)|_{dX \rightarrow Y} = \sum_{i,j} \sum_{k,l} \frac{\partial^2 g_{mn}(X)}{\partial X_{kl} \partial X_{ij}} Y_{kl} Y_{ij} = \text{tr} \left(\nabla_X \text{tr}(\nabla g_{mn}(X)^T Y)^T Y \right) \quad (2019)$$

$$= \sum_{i,j} \lim_{\Delta t \rightarrow 0} \frac{\partial g_{mn}(X + \Delta t Y) - \partial g_{mn}(X)}{\partial X_{ij} \Delta t} Y_{ij} \quad (2020)$$

$$= \lim_{\Delta t \rightarrow 0} \frac{g_{mn}(X + 2\Delta t Y) - 2g_{mn}(X + \Delta t Y) + g_{mn}(X)}{\Delta t^2} \quad (2021)$$

$$= \frac{d^2}{dt^2} \Big|_{t=0} g_{mn}(X + t Y) \quad (2022)$$

Hence the second directional derivative,

$$\begin{aligned} \vec{Y} dg^2(X) &\triangleq \left[\begin{array}{cccc} d^2g_{11}(X) & d^2g_{12}(X) & \cdots & d^2g_{1N}(X) \\ d^2g_{21}(X) & d^2g_{22}(X) & \cdots & d^2g_{2N}(X) \\ \vdots & \vdots & & \vdots \\ d^2g_{M1}(X) & d^2g_{M2}(X) & \cdots & d^2g_{MN}(X) \end{array} \right] \Big|_{dX \rightarrow Y} \in \mathbb{R}^{M \times N} \\ &= \left[\begin{array}{cccc} \text{tr}(\nabla \text{tr}(\nabla g_{11}(X)^T Y)^T Y) & \text{tr}(\nabla \text{tr}(\nabla g_{12}(X)^T Y)^T Y) & \cdots & \text{tr}(\nabla \text{tr}(\nabla g_{1N}(X)^T Y)^T Y) \\ \text{tr}(\nabla \text{tr}(\nabla g_{21}(X)^T Y)^T Y) & \text{tr}(\nabla \text{tr}(\nabla g_{22}(X)^T Y)^T Y) & \cdots & \text{tr}(\nabla \text{tr}(\nabla g_{2N}(X)^T Y)^T Y) \\ \vdots & \vdots & & \vdots \\ \text{tr}(\nabla \text{tr}(\nabla g_{M1}(X)^T Y)^T Y) & \text{tr}(\nabla \text{tr}(\nabla g_{M2}(X)^T Y)^T Y) & \cdots & \text{tr}(\nabla \text{tr}(\nabla g_{MN}(X)^T Y)^T Y) \end{array} \right] \\ &= \left[\begin{array}{cccc} \sum_{i,j} \sum_{k,l} \frac{\partial^2 g_{11}(X)}{\partial X_{kl} \partial X_{ij}} Y_{kl} Y_{ij} & \sum_{i,j} \sum_{k,l} \frac{\partial^2 g_{12}(X)}{\partial X_{kl} \partial X_{ij}} Y_{kl} Y_{ij} & \cdots & \sum_{i,j} \sum_{k,l} \frac{\partial^2 g_{1N}(X)}{\partial X_{kl} \partial X_{ij}} Y_{kl} Y_{ij} \\ \sum_{i,j} \sum_{k,l} \frac{\partial^2 g_{21}(X)}{\partial X_{kl} \partial X_{ij}} Y_{kl} Y_{ij} & \sum_{i,j} \sum_{k,l} \frac{\partial^2 g_{22}(X)}{\partial X_{kl} \partial X_{ij}} Y_{kl} Y_{ij} & \cdots & \sum_{i,j} \sum_{k,l} \frac{\partial^2 g_{2N}(X)}{\partial X_{kl} \partial X_{ij}} Y_{kl} Y_{ij} \\ \vdots & \vdots & & \vdots \\ \sum_{i,j} \sum_{k,l} \frac{\partial^2 g_{M1}(X)}{\partial X_{kl} \partial X_{ij}} Y_{kl} Y_{ij} & \sum_{i,j} \sum_{k,l} \frac{\partial^2 g_{M2}(X)}{\partial X_{kl} \partial X_{ij}} Y_{kl} Y_{ij} & \cdots & \sum_{i,j} \sum_{k,l} \frac{\partial^2 g_{MN}(X)}{\partial X_{kl} \partial X_{ij}} Y_{kl} Y_{ij} \end{array} \right] \quad (2023) \end{aligned}$$

from which it follows

$$\vec{Y} dg^2(X) = \sum_{i,j} \sum_{k,l} \frac{\partial^2 g(X)}{\partial X_{kl} \partial X_{ij}} Y_{kl} Y_{ij} = \sum_{i,j} \frac{\partial}{\partial X_{ij}} \vec{Y} dg(X) Y_{ij} \quad (2024)$$

Yet for all $X \in \text{dom } g$, any $Y \in \mathbb{R}^{K \times L}$, and some open interval of $t \in \mathbb{R}$

$$g(X + t Y) = g(X) + t \vec{Y} dg(X) + \frac{1}{2!} t^2 \vec{Y} dg^2(X) + O(t^3) \quad (2025)$$

which is the second-order multidimensional Taylor series expansion about X . [393, §18.4] [177, §2.3.4] Differentiating twice with respect to t and subsequent t -zeroing isolates the third term of the expansion. Thus differentiating and zeroing $g(X + t Y)$ in t is an operation equivalent to individually differentiating and zeroing every entry $g_{mn}(X + t Y)$ as in (2022). So the second directional derivative of $g(X): \mathbb{R}^{K \times L} \rightarrow \mathbb{R}^{M \times N}$ becomes [315, §2.1, §5.4.5] [36, §6.3.1]

$$\vec{Y} dg^2(X) = \frac{d^2}{dt^2} \Big|_{t=0} g(X + t Y) \in \mathbb{R}^{M \times N} \quad (2026)$$

which is again simplest. (*confer* (2005)) Directional derivative retains the dimensions of g .

D.1.6 directional derivative expressions

In the case of a real function $g(X) : \mathbb{R}^{K \times L} \rightarrow \mathbb{R}$, all its directional derivatives are in \mathbb{R} :

$$\vec{dg}(X) = \text{tr}(\nabla g(X)^T Y) \quad (2027)$$

$$\vec{dg}^2(X) = \text{tr}\left(\nabla_X \text{tr}(\nabla g(X)^T Y)^T Y\right) = \text{tr}\left(\nabla_X \vec{dg}(X)^T Y\right) \quad (2028)$$

$$\vec{dg}^3(X) = \text{tr}\left(\nabla_X \text{tr}\left(\nabla_X \text{tr}(\nabla g(X)^T Y)^T Y\right)^T Y\right) = \text{tr}\left(\nabla_X \vec{dg}^2(X)^T Y\right) \quad (2029)$$

In the case $g(X) : \mathbb{R}^K \rightarrow \mathbb{R}$ has vector argument, they further simplify:

$$\vec{dg}(X) = \nabla g(X)^T Y \quad (2030)$$

$$\vec{dg}^2(X) = Y^T \nabla^2 g(X) Y \quad (2031)$$

$$\vec{dg}^3(X) = \nabla_X (Y^T \nabla^2 g(X) Y)^T Y \quad (2032)$$

and so on.

D.1.7 higher-order multidimensional Taylor series

Series expansions of the differentiable matrix-valued function $g(X)$, of matrix argument, were given earlier in (2004) and (2025). Assume that $g(X)$ has continuous first-, second-, and third-order gradients over open set $\text{dom } g$. Then, for $X \in \text{dom } g$ and any $Y \in \mathbb{R}^{K \times L}$, the Taylor series is expressed on some open interval of $\mu \in \mathbb{R}$

$$g(X + \mu Y) = g(X) + \mu \vec{dg}(X) + \frac{1}{2!} \mu^2 \vec{dg}^2(X) + \frac{1}{3!} \mu^3 \vec{dg}^3(X) + O(\mu^4) \quad (2033)$$

or on some open interval of $\|Y\|_2$

$$g(Y) = g(X) + \vec{dg}(X)^{Y-X} + \frac{1}{2!} \vec{dg}^2(X)^{Y-X} + \frac{1}{3!} \vec{dg}^3(X)^{Y-X} + O(\|Y\|^4) \quad (2034)$$

which are third-order expansions about X . The *mean value theorem* from calculus is what insures finite order of the series. [393] [44, §1.1] [43, App.A.5] [230, §0.4] These somewhat unbelievable formulae^{D.3} imply that a function can be determined over the whole of its domain by knowing its value and all its directional derivatives at a single point X .

D.1.7.0.1 Example. Inverse-matrix function.

Say $g(Y) = Y^{-1}$. From the table on page 566,

$$\vec{dg}(X) = \frac{d}{dt} \Big|_{t=0} g(X + tY) = -X^{-1} Y X^{-1} \quad (2035)$$

$$\vec{dg}^2(X) = \frac{d^2}{dt^2} \Big|_{t=0} g(X + tY) = 2X^{-1} Y X^{-1} Y X^{-1} \quad (2036)$$

^{D.3} e.g., real continuous and differentiable function of real variable $f(x) = e^{-1/x^2}$ has no Taylor series expansion about $x=0$, of any practical use, because each derivative equals 0 there.

$$\frac{\rightarrow Y}{dg^3}(X) = \frac{d^3}{dt^3} \Big|_{t=0} g(X+tY) = -6X^{-1}YX^{-1}YX^{-1}YX^{-1} \quad (2037)$$

Let's find the Taylor series expansion of g about $X=I$: Since $g(I)=I$, for $\|Y\|_2 < 1$ ($\mu=1$ in (2033))

$$g(I+Y) = (I+Y)^{-1} = I - Y + Y^2 - Y^3 + \dots \quad (2038)$$

If Y is small, $(I+Y)^{-1} \approx I - Y$.^{D.4} Now we find Taylor series expansion about X :

$$g(X+Y) = (X+Y)^{-1} = X^{-1} - X^{-1}YX^{-1} + 2X^{-1}YX^{-1}YX^{-1} - \dots \quad (2039)$$

If Y is small, $(X+Y)^{-1} \approx X^{-1} - X^{-1}YX^{-1}$. \square

D.1.7.0.2 Exercise. *log det.*

(confer [66, p.644])

Find the first three terms of a Taylor series expansion for $\log \det Y$. Specify an open interval over which the expansion holds in vicinity of X . \blacktriangledown

D.1.8 Correspondence of gradient to derivative

From the foregoing expressions for directional derivative, we derive a relationship between gradient with respect to matrix X and derivative with respect to real variable t :

D.1.8.1 first-order

Removing evaluation at $t=0$ from (2005),^{D.5} we find an expression for the directional derivative of $g(X)$ in direction Y evaluated anywhere along a line $\{X+tY \mid t \in \mathbb{R}\}$ intersecting $\text{dom } g$

$$\frac{\rightarrow Y}{dg}(X+tY) = \frac{d}{dt}g(X+tY) \quad (2040)$$

In the general case $g(X) : \mathbb{R}^{K \times L} \rightarrow \mathbb{R}^{M \times N}$, from (1998) and (2001) we find

$$\text{tr}(\nabla_X g_{mn}(X+tY)^T Y) = \frac{d}{dt}g_{mn}(X+tY) \quad (2041)$$

which is valid at $t=0$, of course, when $X \in \text{dom } g$. In the important case of a real function $g(X) : \mathbb{R}^{K \times L} \rightarrow \mathbb{R}$, from (2027) we have simply

$$\text{tr}(\nabla_X g(X+tY)^T Y) = \frac{d}{dt}g(X+tY) \quad (2042)$$

When $g(X) : \mathbb{R}^K \rightarrow \mathbb{R}$ has vector argument,

$$\nabla_X g(X+tY)^T Y = \frac{d}{dt}g(X+tY) \quad (2043)$$

^{D.4}Had we instead set $g(Y)=(I+Y)^{-1}$, then the equivalent expansion would have been about $X=0$.

^{D.5}Justified by replacing X with $X+tY$ in (1998)-(2000); beginning,

$$dg_{mn}(X+tY)|_{dX \rightarrow Y} = \sum_{k,l} \frac{\partial g_{mn}(X+tY)}{\partial X_{kl}} Y_{kl}$$

D.1.8.1.1 Example. *Gradient.*

$g(X) = w^T X^T X w$, $X \in \mathbb{R}^{K \times L}$, $w \in \mathbb{R}^L$. Using the tables in §D.2,

$$\text{tr}(\nabla_X g(X + tY)^T Y) = \text{tr}(2ww^T(X^T + tY^T)Y) \quad (2044)$$

$$= 2w^T(X^T Y + tY^T Y)w \quad (2045)$$

Applying equivalence (2042),

$$\frac{d}{dt}g(X + tY) = \frac{d}{dt}w^T(X + tY)^T(X + tY)w \quad (2046)$$

$$= w^T(X^T Y + Y^T X + 2tY^T Y)w \quad (2047)$$

$$= 2w^T(X^T Y + tY^T Y)w \quad (2048)$$

which is the same as (2045). Hence, the equivalence is demonstrated.

It is easy to extract $\nabla g(X)$ from (2048) knowing only (2042):

$$\begin{aligned} \text{tr}(\nabla_X g(X + tY)^T Y) &= 2w^T(X^T Y + tY^T Y)w \\ &= 2\text{tr}(ww^T(X^T + tY^T)Y) \\ \text{tr}(\nabla_X g(X)^T Y) &= 2\text{tr}(ww^T X^T Y) \\ &\Leftrightarrow \\ \nabla_X g(X) &= 2Xww^T \end{aligned} \quad (2049)$$

□

D.1.8.2 second-order

Likewise removing the evaluation at $t = 0$ from (2026),

$$\vec{d}g^2(X + tY) = \frac{d^2}{dt^2}g(X + tY) \quad (2050)$$

we can find a similar relationship between second-order gradient and second derivative: In the general case $g(X) : \mathbb{R}^{K \times L} \rightarrow \mathbb{R}^{M \times N}$ from (2019) and (2022),

$$\text{tr}(\nabla_X \text{tr}(\nabla_X g_{mn}(X + tY)^T Y)) = \frac{d^2}{dt^2}g_{mn}(X + tY) \quad (2051)$$

In the case of a real function $g(X) : \mathbb{R}^{K \times L} \rightarrow \mathbb{R}$ we have, of course,

$$\text{tr}(\nabla_X \text{tr}(\nabla_X g(X + tY)^T Y)) = \frac{d^2}{dt^2}g(X + tY) \quad (2052)$$

From (2031), the simpler case, where real function $g(X) : \mathbb{R}^K \rightarrow \mathbb{R}$ has vector argument,

$$Y^T \nabla_X^2 g(X + tY) Y = \frac{d^2}{dt^2}g(X + tY) \quad (2053)$$

D.1.8.2.1 Example. *Second-order gradient.*

We want to find $\nabla^2 g(X) \in \mathbb{R}^{K \times K \times K \times K}$ given real function $g(X) = \log \det X$ having domain $\text{intr } \mathbb{S}_+^K$. From the tables in §D.2,

$$h(X) \triangleq \nabla g(X) = X^{-1} \in \text{intr } \mathbb{S}_+^K \quad (2054)$$

so $\nabla^2 g(X) = \nabla h(X)$. By (2041) and (2004), for $Y \in \mathbb{S}^K$

$$\text{tr}(\nabla h_{mn}(X)^T Y) = \left. \frac{d}{dt} \right|_{t=0} h_{mn}(X + tY) \quad (2055)$$

$$= \left(\left. \frac{d}{dt} \right|_{t=0} h(X + tY) \right)_{mn} \quad (2056)$$

$$= \left(\left. \frac{d}{dt} \right|_{t=0} (X + tY)^{-1} \right)_{mn} \quad (2057)$$

$$= -(X^{-1} Y X^{-1})_{mn} \quad (2058)$$

Setting Y to a member of $\{e_k e_l^T \in \mathbb{R}^{K \times K} \mid k, l = 1 \dots K\}$, and employing a property (41) of the trace function we find

$$\nabla^2 g(X)_{mnkl} = \text{tr}(\nabla h_{mn}(X)^T e_k e_l^T) = \nabla h_{mn}(X)_{kl} = -(X^{-1} e_k e_l^T X^{-1})_{mn} \quad (2059)$$

$$\nabla^2 g(X)_{kl} = \nabla h(X)_{kl} = -(X^{-1} e_k e_l^T X^{-1}) \in \mathbb{R}^{K \times K} \quad (2060)$$

□

From all these first- and second-order expressions, we may generate new ones by evaluating both sides at arbitrary t (in some open interval) but only after differentiation.

D.2 Tables of gradients and derivatives

- Results may be validated numerically via *Richardson extrapolation*. [280, §5.4] [122] When algebraically proving results for symmetric matrices, it is critical to take gradients ignoring symmetry and to then substitute symmetric entries afterward. [194] [70]
- $i, j, k, \ell, K, L, m, n, M, N$ are integers, unless otherwise noted, $a, b \in \mathbb{R}^n$, $x, y \in \mathbb{R}^k$, $A, B \in \mathbb{R}^{m \times n}$, $X, Y \in \mathbb{R}^{K \times L}$, $t, \mu \in \mathbb{R}$.
- x^μ means $\delta(\delta(x)^\mu)$ for $\mu \in \mathbb{R}$; *id est*, entrywise vector exponentiation. δ is the main-diagonal linear operator (1585). $x^0 \triangleq \mathbf{1}$, $X^0 \triangleq I$ if square.
- $\frac{d}{dx} \triangleq \begin{bmatrix} \frac{d}{dx_1} \\ \vdots \\ \frac{d}{dx_k} \end{bmatrix}$, $\overset{\rightarrow y}{dg}(x)$, $\overset{\rightarrow y}{dg^2}(x)$ (directional derivatives §D.1), $\log x$, e^x , $|x|$, x/y (Hadamard quotient), $\text{sgn } x$, $\sqrt[k]{x}$ (entrywise square root), *etcetera*, are maps $f : \mathbb{R}^k \rightarrow \mathbb{R}^k$ that maintain dimension; e.g., (§A.1.1)

$$\frac{d}{dx} x^{-1} \triangleq \nabla_x \mathbf{1}^T \delta(x)^{-1} \mathbf{1} \quad (2061)$$

- For A a scalar or square matrix, we have the Taylor series [84, §3.6]

$$e^A \triangleq \sum_{k=0}^{\infty} \frac{1}{k!} A^k \quad (2062)$$

Further, [374, §5.4]

$$e^A \succ 0 \quad \forall A \in \mathbb{S}^m \quad (2063)$$

- For all square A and integer k

$$\det^k A = \det A^k \quad (2064)$$

algebraic continued

$$\frac{d}{dt}(X + tY) = Y$$

$$\frac{d}{dt}B^T(X + tY)^{-1}A = -B^T(X + tY)^{-1}Y(X + tY)^{-1}A$$

$$\frac{d}{dt}B^T(X + tY)^{-T}A = -B^T(X + tY)^{-T}Y^T(X + tY)^{-T}A$$

$$\frac{d}{dt}B^T(X + tY)^\mu A = \dots, \quad -1 \leq \mu \leq 1, \quad X, Y \in \mathbb{S}_+^M$$

$$\frac{d^2}{dt^2}B^T(X + tY)^{-1}A = -2B^T(X + tY)^{-1}Y(X + tY)^{-1}Y(X + tY)^{-1}A$$

$$\frac{d^3}{dt^3}B^T(X + tY)^{-1}A = -6B^T(X + tY)^{-1}Y(X + tY)^{-1}Y(X + tY)^{-1}Y(X + tY)^{-1}A$$

$$\frac{d}{dt}((X + tY)^T A (X + tY)) = Y^T A X + X^T A Y + 2t Y^T A Y$$

$$\frac{d^2}{dt^2}((X + tY)^T A (X + tY)) = 2Y^T A Y$$

$$\begin{aligned} \frac{d}{dt}((X + tY)^T A (X + tY))^{-1} \\ = -((X + tY)^T A (X + tY))^{-1} (Y^T A X + X^T A Y + 2t Y^T A Y) ((X + tY)^T A (X + tY))^{-1} \end{aligned}$$

$$\frac{d}{dt}((X + tY) A (X + tY)) = Y A X + X A Y + 2t Y A Y$$

$$\frac{d^2}{dt^2}((X + tY) A (X + tY)) = 2Y A Y$$

D.2.2 trace Kronecker

$$\nabla_{\text{vec } X} \text{tr}(A X B X^T) = \nabla_{\text{vec } X} \text{vec}(X)^T (B^T \otimes A) \text{vec } X = (B \otimes A^T + B^T \otimes A) \text{vec } X$$

$$\nabla_{\text{vec } X}^2 \text{tr}(A X B X^T) = \nabla_{\text{vec } X}^2 \text{vec}(X)^T (B^T \otimes A) \text{vec } X = B \otimes A^T + B^T \otimes A \quad (1977)$$

D.2.3 trace

$\nabla_x \mu x = \mu I$	$\nabla_X \operatorname{tr} \mu X = \nabla_X \mu \operatorname{tr} X = \mu I$
$\nabla_x \mathbf{1}^T \delta(x)^{-1} \mathbf{1} = \frac{d}{dx} x^{-1} = -x^{-2}$	$\nabla_X \operatorname{tr} X^{-1} = -X^{-2T}$
$\nabla_x \mathbf{1}^T \delta(x)^{-1} y = -\delta(x)^{-2} y$	$\nabla_X \operatorname{tr}(X^{-1} Y) = \nabla_X \operatorname{tr}(Y X^{-1}) = -X^{-T} Y^T X^{-T}$
$\frac{d}{dx} x^\mu = \mu x^{\mu-1}$	$\nabla_X \operatorname{tr} X^\mu = \mu X^{\mu-1}, \quad X \in \mathbb{S}^M$
	$\nabla_X \operatorname{tr} X^j = j X^{(j-1)T}$
$\nabla_x (b - a^T x)^{-1} = (b - a^T x)^{-2} a$	$\nabla_X \operatorname{tr}((B - AX)^{-1}) = ((B - AX)^{-2} A)^T$
$\nabla_x (b - a^T x)^\mu = -\mu (b - a^T x)^{\mu-1} a$	
$\nabla_x x^T y = \nabla_x y^T x = y$	$\nabla_X \operatorname{tr}(X^T Y) = \nabla_X \operatorname{tr}(Y X^T) = \nabla_X \operatorname{tr}(Y^T X) = \nabla_X \operatorname{tr}(X Y^T) = Y$
$\nabla_x x^T x = 2x$	$\nabla_X \operatorname{tr}(X^T X) = \nabla_X \operatorname{tr}(X X^T) = 2X$
	$\nabla_X \operatorname{tr}(AXBX^T) = \nabla_X \operatorname{tr}(XBX^T A) = A^T X B^T + A X B$
	$\nabla_X \operatorname{tr}(AXBX) = \nabla_X \operatorname{tr}(XBX A) = A^T X^T B^T + B^T X^T A^T$
	$\nabla_X \operatorname{tr}(AXAXAXAX) = \nabla_X \operatorname{tr}(XAXAXAXA) = 4(AXAXAXA)^T$
	$\nabla_X \operatorname{tr}(AXAXAX) = \nabla_X \operatorname{tr}(XAXAXA) = 3(AXAXA)^T$
	$\nabla_X \operatorname{tr}(AXAX) = \nabla_X \operatorname{tr}(XAXA) = 2(AXA)^T$
	$\nabla_X \operatorname{tr}(AX) = \nabla_X \operatorname{tr}(XA) = A^T$
	$\nabla_X \operatorname{tr}(Y X^k) = \nabla_X \operatorname{tr}(X^k Y) = \sum_{i=0}^{k-1} (X^i Y X^{k-1-i})^T$
	$\nabla_X \operatorname{tr}(X^T Y Y^T X X^T Y Y^T X) = 4Y Y^T X X^T Y Y^T X$
	$\nabla_X \operatorname{tr}(X Y Y^T X^T X Y Y^T X^T) = 4X Y Y^T X^T X Y Y^T$
	$\nabla_X \operatorname{tr}(Y^T X X^T Y) = \nabla_X \operatorname{tr}(X^T Y Y^T X) = 2Y Y^T X$
	$\nabla_X \operatorname{tr}(Y^T X^T X Y) = \nabla_X \operatorname{tr}(X Y Y^T X^T) = 2X Y Y^T$
	$\nabla_X \operatorname{tr}((X + Y)^T (X + Y)) = 2(X + Y) = \nabla_X \ X + Y\ _F^2$
	$\nabla_X \operatorname{tr}((X + Y)(X + Y)) = 2(X + Y)^T$
	$\nabla_X \operatorname{tr}(A^T X B) = \nabla_X \operatorname{tr}(X^T A B^T) = A B^T$
	$\nabla_X \operatorname{tr}(A^T X^{-1} B) = \nabla_X \operatorname{tr}(X^{-T} A B^T) = -X^{-T} A B^T X^{-T}$
	$\nabla_X a^T X b = \nabla_X \operatorname{tr}(b a^T X) = \nabla_X \operatorname{tr}(X b a^T) = a b^T$
	$\nabla_X b^T X^T a = \nabla_X \operatorname{tr}(X^T a b^T) = \nabla_X \operatorname{tr}(a b^T X^T) = a b^T$
	$\nabla_X a^T X^{-1} b = \nabla_X \operatorname{tr}(X^{-T} a b^T) = -X^{-T} a b^T X^{-T}$
	$\nabla_X a^T X^\mu b = \dots$

trace continued

$$\frac{d}{dt} \operatorname{tr} g(X + tY) = \operatorname{tr} \frac{d}{dt} g(X + tY) \quad [234, \text{p.491}]$$

$$\frac{d}{dt} \operatorname{tr}(X + tY) = \operatorname{tr} Y$$

$$\frac{d}{dt} \operatorname{tr}^j(X + tY) = j \operatorname{tr}^{j-1}(X + tY) \operatorname{tr} Y$$

$$\frac{d}{dt} \operatorname{tr}(X + tY)^j = j \operatorname{tr}((X + tY)^{j-1} Y) \quad (\forall j)$$

$$\frac{d}{dt} \operatorname{tr}((X + tY)Y) = \operatorname{tr} Y^2$$

$$\frac{d}{dt} \operatorname{tr}((X + tY)^k Y) = \frac{d}{dt} \operatorname{tr}(Y(X + tY)^k) = k \operatorname{tr}((X + tY)^{k-1} Y^2), \quad k \in \{0, 1, 2\}$$

$$\frac{d}{dt} \operatorname{tr}((X + tY)^k Y) = \frac{d}{dt} \operatorname{tr}(Y(X + tY)^k) = \operatorname{tr} \sum_{i=0}^{k-1} (X + tY)^i Y (X + tY)^{k-1-i}$$

$$\begin{aligned} \frac{d}{dt} \operatorname{tr}((X + tY)^{-1} Y) &= -\operatorname{tr}((X + tY)^{-1} Y (X + tY)^{-1} Y) \\ \frac{d}{dt} \operatorname{tr}(B^T (X + tY)^{-1} A) &= -\operatorname{tr}(B^T (X + tY)^{-1} Y (X + tY)^{-1} A) \\ \frac{d}{dt} \operatorname{tr}(B^T (X + tY)^{-T} A) &= -\operatorname{tr}(B^T (X + tY)^{-T} Y^T (X + tY)^{-T} A) \\ \frac{d}{dt} \operatorname{tr}(B^T (X + tY)^{-k} A) &= \dots, \quad k > 0 \\ \frac{d}{dt} \operatorname{tr}(B^T (X + tY)^\mu A) &= \dots, \quad -1 \leq \mu \leq 1, \quad X, Y \in \mathbb{S}_+^M \end{aligned}$$

$$\frac{d^2}{dt^2} \operatorname{tr}(B^T (X + tY)^{-1} A) = 2 \operatorname{tr}(B^T (X + tY)^{-1} Y (X + tY)^{-1} Y (X + tY)^{-1} A)$$

$$\frac{d}{dt} \operatorname{tr}((X + tY)^T A (X + tY)) = \operatorname{tr}(Y^T A X + X^T A Y + 2t Y^T A Y)$$

$$\frac{d^2}{dt^2} \operatorname{tr}((X + tY)^T A (X + tY)) = 2 \operatorname{tr}(Y^T A Y)$$

$$\begin{aligned} \frac{d}{dt} \operatorname{tr}(((X + tY)^T A (X + tY))^{-1}) \\ = -\operatorname{tr}(((X + tY)^T A (X + tY))^{-1} (Y^T A X + X^T A Y + 2t Y^T A Y) ((X + tY)^T A (X + tY))^{-1}) \end{aligned}$$

$$\frac{d}{dt} \operatorname{tr}((X + tY) A (X + tY)) = \operatorname{tr}(Y A X + X A Y + 2t Y A Y)$$

$$\frac{d^2}{dt^2} \operatorname{tr}((X + tY) A (X + tY)) = 2 \operatorname{tr}(Y A Y)$$

D.2.4 logarithmic determinant

$x \succ 0$, $\det X > 0$ on some neighborhood of X , and $\det(X + tY) > 0$ on some open interval of t ; otherwise, $\log(\cdot)$ would be discontinuous. [91, p.75]

$\frac{d}{dx} \log x = x^{-1}$	$\nabla_X \log \det X = X^{-T}$
	$\nabla_X^2 \log \det(X)_{kl} = \frac{\partial X^{-T}}{\partial X_{kl}} = -(X^{-1} e_k e_l^T X^{-1})^T$, <i>confer</i> (2013)(2060)
$\frac{d}{dx} \log x^{-1} = -x^{-1}$	$\nabla_X \log \det X^{-1} = -X^{-T}$
$\frac{d}{dx} \log x^\mu = \mu x^{-1}$	$\nabla_X \log \det^\mu X = \mu X^{-T}$
	$\nabla_X \log \det X^\mu = \mu X^{-T}$
	$\nabla_X \log \det X^k = \nabla_X \log \det^k X = k X^{-T}$
	$\nabla_X \log \det^\mu(X + tY) = \mu(X + tY)^{-T}$
$\nabla_x \log(a^T x + b) = a \frac{1}{a^T x + b}$	$\nabla_X \log \det(AX + B) = A^T(AX + B)^{-T}$
	$\nabla_X \log \det(I \pm A^T X A) = \pm A(I \pm A^T X A)^{-T} A^T$
	$\nabla_X \log \det(X + tY)^k = \nabla_X \log \det^k(X + tY) = k(X + tY)^{-T}$
	$\frac{d}{dt} \log \det(X + tY) = \text{tr}((X + tY)^{-1} Y)$
	$\frac{d^2}{dt^2} \log \det(X + tY) = -\text{tr}((X + tY)^{-1} Y (X + tY)^{-1} Y)$
	$\frac{d}{dt} \log \det(X + tY)^{-1} = -\text{tr}((X + tY)^{-1} Y)$
	$\frac{d^2}{dt^2} \log \det(X + tY)^{-1} = \text{tr}((X + tY)^{-1} Y (X + tY)^{-1} Y)$
	$\frac{d}{dt} \log \det(\delta(A(x + ty) + a)^2 + \mu I)$ $= \text{tr}\left((\delta(A(x + ty) + a)^2 + \mu I)^{-1} 2\delta(A(x + ty) + a)\delta(Ay)\right)$

D.2.5 determinant

$$\begin{aligned}
\nabla_X \det X &= \nabla_X \det X^T = \det(X) X^{-T} \\
\nabla_X \det X^{-1} &= -\det(X^{-1}) X^{-T} = -\det(X)^{-1} X^{-T} \\
\nabla_X \det^\mu X &= \mu \det^\mu(X) X^{-T} \\
\nabla_X \det X^\mu &= \mu \det(X^\mu) X^{-T} \\
\nabla_X \det X^k &= k \det^{k-1}(X) (\operatorname{tr}(X) I - X^T) , & X \in \mathbb{R}^{2 \times 2} \\
\nabla_X \det X^k &= \nabla_X \det^k X = k \det(X^k) X^{-T} = k \det^k(X) X^{-T} \\
\nabla_X \det^\mu(X + tY) &= \mu \det^\mu(X + tY) (X + tY)^{-T} \\
\nabla_X \det(X + tY)^k &= \nabla_X \det^k(X + tY) = k \det^k(X + tY) (X + tY)^{-T} \\
\frac{d}{dt} \det(X + tY) &= \det(X + tY) \operatorname{tr}((X + tY)^{-1} Y) \\
\frac{d^2}{dt^2} \det(X + tY) &= \det(X + tY) (\operatorname{tr}^2((X + tY)^{-1} Y) - \operatorname{tr}((X + tY)^{-1} Y (X + tY)^{-1} Y)) \\
\frac{d}{dt} \det(X + tY)^{-1} &= -\det(X + tY)^{-1} \operatorname{tr}((X + tY)^{-1} Y) \\
\frac{d^2}{dt^2} \det(X + tY)^{-1} &= \det(X + tY)^{-1} (\operatorname{tr}^2((X + tY)^{-1} Y) + \operatorname{tr}((X + tY)^{-1} Y (X + tY)^{-1} Y)) \\
\frac{d}{dt} \det^\mu(X + tY) &= \mu \det^\mu(X + tY) \operatorname{tr}((X + tY)^{-1} Y)
\end{aligned}$$

D.2.6 logarithmic

Matrix logarithm.

$$\begin{aligned}
\frac{d}{dt} \log(X + tY)^\mu &= \mu Y (X + tY)^{-1} = \mu (X + tY)^{-1} Y , & XY = YX \\
\frac{d}{dt} \log(I - tY)^\mu &= -\mu Y (I - tY)^{-1} = -\mu (I - tY)^{-1} Y & [234, \text{p.493}]
\end{aligned}$$

D.2.7 exponential

Matrix exponential. [84, §3.6, §4.5] [374, §5.4]

$$\nabla_X e^{\text{tr}(Y^T X)} = \nabla_X \det e^{Y^T X} = e^{\text{tr}(Y^T X)} Y \quad (\forall X, Y)$$

$$\begin{aligned} \nabla_X \text{tr} e^{YX} &= e^{Y^T X^T} Y^T = Y^T e^{X^T Y^T} \\ \nabla_X \text{tr}(A e^{YX}) &= \dots \end{aligned} \quad (\forall X, Y)$$

$$\nabla_x \mathbf{1}^T e^{Ax} = A^T e^{Ax}$$

$$\nabla_x \mathbf{1}^T e^{|Ax|} = A^T \delta(\text{sgn}(Ax)) e^{|Ax|} \quad (Ax)_i \neq 0$$

$$\nabla_x \log(\mathbf{1}^T e^x) = \frac{1}{\mathbf{1}^T e^x} e^x$$

$$\nabla_x^2 \log(\mathbf{1}^T e^x) = \frac{1}{\mathbf{1}^T e^x} \left(\delta(e^x) - \frac{1}{\mathbf{1}^T e^x} e^x e^{x^T} \right)$$

$$\nabla_x \prod_{i=1}^k x_i^{\frac{1}{k}} = \frac{1}{k} \left(\prod_{i=1}^k x_i^{\frac{1}{k}} \right) \mathbf{1}/x$$

$$\nabla_x^2 \prod_{i=1}^k x_i^{\frac{1}{k}} = -\frac{1}{k} \left(\prod_{i=1}^k x_i^{\frac{1}{k}} \right) \left(\delta(x)^{-2} - \frac{1}{k} (\mathbf{1}/x)(\mathbf{1}/x)^T \right)$$

$$\frac{d}{dt} e^{tY} = e^{tY} Y = Y e^{tY}$$

$$\frac{d}{dt} e^{X+tY} = e^{X+tY} Y = Y e^{X+tY}, \quad XY = YX$$

$$\frac{d^2}{dt^2} e^{X+tY} = e^{X+tY} Y^2 = Y e^{X+tY} Y = Y^2 e^{X+tY}, \quad XY = YX$$

$$\frac{d^j}{dt^j} e^{\text{tr}(X+tY)} = e^{\text{tr}(X+tY)} \text{tr}^j(Y)$$

D.2.7.0.1 Exercise. Expand these tables.

Provide four unfinished table entries indicated by ... in §D.2.1 & §D.2.3. ▼

D.2.7.0.2 Exercise. \log .

(§D.1.7, §3.5.4)

Find the first four terms of the Taylor series expansion for $\log x$ about $x = 1$. Plot the supporting hyperplane to the hypograph of $\log x$ at $\begin{bmatrix} x \\ \log x \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$. Prove $\log x \leq x - 1$. ▼