

Appendix D

Matrix calculus

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

—Isaac Newton [86, §5]

D.1 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 domain is defined

$$\nabla f(x) \triangleq \begin{bmatrix} \frac{\partial f(x)}{\partial x_1} \\ \frac{\partial f(x)}{\partial x_2} \\ \vdots \\ \frac{\partial f(x)}{\partial x_K} \end{bmatrix} \in \mathbb{R}^K \quad (1354)$$

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

$$\nabla^2 f(x) \triangleq \begin{bmatrix} \frac{\partial^2 f(x)}{\partial^2 x_1} & \frac{\partial^2 f(x)}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_1 \partial x_K} \\ \frac{\partial^2 f(x)}{\partial x_2 \partial x_1} & \frac{\partial^2 f(x)}{\partial^2 x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_2 \partial x_K} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f(x)}{\partial x_K \partial x_1} & \frac{\partial^2 f(x)}{\partial x_K \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial^2 x_K} \end{bmatrix} \in \mathbb{S}^K \quad (1355)$$

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

$$\nabla v(x) \triangleq \left[\frac{\partial v_1(x)}{\partial x} \quad \frac{\partial v_2(x)}{\partial x} \quad \dots \quad \frac{\partial v_N(x)}{\partial x} \right] \in \mathbb{R}^N \quad (1356)$$

while the second-order gradient is

$$\nabla^2 v(x) \triangleq \left[\frac{\partial^2 v_1(x)}{\partial x^2} \quad \frac{\partial^2 v_2(x)}{\partial x^2} \quad \dots \quad \frac{\partial^2 v_N(x)}{\partial x^2} \right] \in \mathbb{R}^N \quad (1357)$$

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

$$\begin{aligned} \nabla h(x) &\triangleq \begin{bmatrix} \frac{\partial h_1(x)}{\partial x_1} & \frac{\partial h_2(x)}{\partial x_1} & \dots & \frac{\partial h_N(x)}{\partial x_1} \\ \frac{\partial h_1(x)}{\partial x_2} & \frac{\partial h_2(x)}{\partial x_2} & \dots & \frac{\partial h_N(x)}{\partial x_2} \\ \vdots & \vdots & & \vdots \\ \frac{\partial h_1(x)}{\partial x_K} & \frac{\partial h_2(x)}{\partial x_K} & \dots & \frac{\partial h_N(x)}{\partial x_K} \end{bmatrix} \\ &= [\nabla h_1(x) \quad \nabla h_2(x) \quad \dots \quad \nabla h_N(x)] \in \mathbb{R}^{K \times N} \end{aligned} \quad (1358)$$

while the second-order gradient has a three-dimensional representation dubbed *cubix* ;^{D.1}

$$\begin{aligned} \nabla^2 h(x) &\triangleq \begin{bmatrix} \nabla \frac{\partial h_1(x)}{\partial x_1} & \nabla \frac{\partial h_2(x)}{\partial x_1} & \dots & \nabla \frac{\partial h_N(x)}{\partial x_1} \\ \nabla \frac{\partial h_1(x)}{\partial x_2} & \nabla \frac{\partial h_2(x)}{\partial x_2} & \dots & \nabla \frac{\partial h_N(x)}{\partial x_2} \\ \vdots & \vdots & & \vdots \\ \nabla \frac{\partial h_1(x)}{\partial x_K} & \nabla \frac{\partial h_2(x)}{\partial x_K} & \dots & \nabla \frac{\partial h_N(x)}{\partial x_K} \end{bmatrix} \\ &= [\nabla^2 h_1(x) \quad \nabla^2 h_2(x) \quad \dots \quad \nabla^2 h_N(x)] \in \mathbb{R}^{K \times N \times K} \end{aligned} \quad (1359)$$

where the gradient of each real entry is with respect to vector x as in (1354).

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

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

$$\begin{aligned}
 \nabla g(X) &\triangleq \begin{bmatrix} \frac{\partial g(X)}{\partial X_{11}} & \frac{\partial g(X)}{\partial X_{12}} & \dots & \frac{\partial g(X)}{\partial X_{1L}} \\ \frac{\partial g(X)}{\partial X_{21}} & \frac{\partial g(X)}{\partial X_{22}} & \dots & \frac{\partial g(X)}{\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \frac{\partial g(X)}{\partial X_{K1}} & \frac{\partial g(X)}{\partial X_{K2}} & \dots & \frac{\partial g(X)}{\partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K \times L} \\
 &= \begin{bmatrix} \nabla_{X(:,1)} g(X) \\ \nabla_{X(:,2)} g(X) \\ \vdots \\ \nabla_{X(:,L)} g(X) \end{bmatrix} \in \mathbb{R}^{K \times 1 \times L}
 \end{aligned} \tag{1360}$$

where the gradient $\nabla_{X(:,i)}$ is with respect to the i^{th} column of X . The strange appearance of (1360) 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

$$\begin{aligned}
 \nabla^2 g(X) &\triangleq \begin{bmatrix} \nabla \frac{\partial g(X)}{\partial X_{11}} & \nabla \frac{\partial g(X)}{\partial X_{12}} & \dots & \nabla \frac{\partial g(X)}{\partial X_{1L}} \\ \nabla \frac{\partial g(X)}{\partial X_{21}} & \nabla \frac{\partial g(X)}{\partial X_{22}} & \dots & \nabla \frac{\partial g(X)}{\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \nabla \frac{\partial g(X)}{\partial X_{K1}} & \nabla \frac{\partial g(X)}{\partial X_{K2}} & \dots & \nabla \frac{\partial g(X)}{\partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K \times L \times K \times L} \\
 &= \begin{bmatrix} \nabla \nabla_{X(:,1)} g(X) \\ \nabla \nabla_{X(:,2)} g(X) \\ \vdots \\ \nabla \nabla_{X(:,L)} g(X) \end{bmatrix} \in \mathbb{R}^{K \times 1 \times L \times K \times L}
 \end{aligned} \tag{1361}$$

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

$$\begin{aligned} \nabla g(X) &\triangleq \begin{bmatrix} \nabla_{X(:,1)} g_1(X) & \nabla_{X(:,1)} g_2(X) & \cdots & \nabla_{X(:,1)} g_N(X) \\ \nabla_{X(:,2)} g_1(X) & \nabla_{X(:,2)} g_2(X) & \cdots & \nabla_{X(:,2)} g_N(X) \\ \vdots & \vdots & \ddots & \vdots \\ \nabla_{X(:,L)} g_1(X) & \nabla_{X(:,L)} g_2(X) & \cdots & \nabla_{X(:,L)} g_N(X) \end{bmatrix} \\ &= [\nabla g_1(X) \quad \nabla g_2(X) \quad \cdots \quad \nabla g_N(X)] \in \mathbb{R}^{K \times N \times L} \end{aligned} \quad (1362)$$

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

$$\begin{aligned} \nabla^2 g(X) &\triangleq \begin{bmatrix} \nabla \nabla_{X(:,1)} g_1(X) & \nabla \nabla_{X(:,1)} g_2(X) & \cdots & \nabla \nabla_{X(:,1)} g_N(X) \\ \nabla \nabla_{X(:,2)} g_1(X) & \nabla \nabla_{X(:,2)} g_2(X) & \cdots & \nabla \nabla_{X(:,2)} g_N(X) \\ \vdots & \vdots & \ddots & \vdots \\ \nabla \nabla_{X(:,L)} g_1(X) & \nabla \nabla_{X(:,L)} g_2(X) & \cdots & \nabla \nabla_{X(:,L)} g_N(X) \end{bmatrix} \\ &= [\nabla^2 g_1(X) \quad \nabla^2 g_2(X) \quad \cdots \quad \nabla^2 g_N(X)] \in \mathbb{R}^{K \times N \times L \times K \times L} \end{aligned} \quad (1363)$$

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*

$$\nabla g(X) \triangleq \begin{bmatrix} \nabla g_{11}(X) & \nabla g_{12}(X) & \cdots & \nabla g_{1N}(X) \\ \nabla g_{21}(X) & \nabla g_{22}(X) & \cdots & \nabla g_{2N}(X) \\ \vdots & \vdots & \ddots & \vdots \\ \nabla g_{M1}(X) & \nabla g_{M2}(X) & \cdots & \nabla g_{MN}(X) \end{bmatrix} \in \mathbb{R}^{M \times N \times K \times L} \quad (1364)$$

while the second-order gradient has six-dimensional representation

$$\nabla^2 g(X) \triangleq \begin{bmatrix} \nabla^2 g_{11}(X) & \nabla^2 g_{12}(X) & \cdots & \nabla^2 g_{1N}(X) \\ \nabla^2 g_{21}(X) & \nabla^2 g_{22}(X) & \cdots & \nabla^2 g_{2N}(X) \\ \vdots & \vdots & \ddots & \vdots \\ \nabla^2 g_{M1}(X) & \nabla^2 g_{M2}(X) & \cdots & \nabla^2 g_{MN}(X) \end{bmatrix} \in \mathbb{R}^{M \times N \times K \times L \times K \times L} \quad (1365)$$

and so on.

D.1.2 Product rules for matrix-functions

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

$$\nabla_X(f(X)^T g(X)) = \nabla_X(f) g + \nabla_X(g) f \quad (1366)$$

while [35, §8.3] [205]

$$\nabla_X \operatorname{tr}(f(X)^T g(X)) = \nabla_X \left(\operatorname{tr}(f(X)^T g(X)) + \operatorname{tr}(g(X) f(X)^T) \right) \Big|_{Z \leftarrow X} \quad (1367)$$

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

$$\nabla_X(f(X)^T g(X)) = \nabla_X a^T X^2 b \quad (1368)$$

using the product rule. Formula (1366) calls for

$$\nabla_X a^T X^2 b = \nabla_X(X^T a) X b + \nabla_X(X b) X^T a \quad (1369)$$

Consider the first of the two terms:

$$\begin{aligned} \nabla_X(f) g &= \nabla_X(X^T a) X b \\ &= \begin{bmatrix} \nabla(X^T a)_1 & \nabla(X^T a)_2 \end{bmatrix} X b \end{aligned} \quad (1370)$$

The gradient of $X^T a$ forms a cubix in $\mathbb{R}^{2 \times 2 \times 2}$.

$$\nabla_X(X^T a) X b = \begin{bmatrix} \frac{\partial(X^T a)_1}{\partial X_{11}} & \dots & \frac{\partial(X^T a)_2}{\partial X_{11}} \\ \vdots & \frac{\partial(X^T a)_1}{\partial X_{12}} & \dots & \frac{\partial(X^T a)_2}{\partial X_{12}} \\ \vdots & \vdots & \frac{\partial(X^T a)_1}{\partial X_{21}} & \dots & \frac{\partial(X^T a)_2}{\partial X_{21}} \\ \vdots & \vdots & \vdots & \frac{\partial(X^T a)_1}{\partial X_{22}} & \dots & \frac{\partial(X^T a)_2}{\partial X_{22}} \end{bmatrix} \begin{bmatrix} (Xb)_1 \\ (Xb)_2 \end{bmatrix} \in \mathbb{R}^{2 \times 1 \times 2} \quad (1371)$$

Because gradient of the product (1368) 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 the second dimension of the cubix (indicated by dotted line segments);

$$\begin{aligned}\nabla_X(X^T a) Xb &= \begin{bmatrix} a_1 & 0 & \\ & 0 & a_1 \\ a_2 & 0 & \\ & 0 & a_2 \end{bmatrix} \begin{bmatrix} b_1 X_{11} + b_2 X_{12} \\ b_1 X_{21} + b_2 X_{22} \end{bmatrix} \in \mathbb{R}^{2 \times 1 \times 2} \\ &= \begin{bmatrix} a_1(b_1 X_{11} + b_2 X_{12}) & a_1(b_1 X_{21} + b_2 X_{22}) \\ a_2(b_1 X_{11} + b_2 X_{12}) & a_2(b_1 X_{21} + b_2 X_{22}) \end{bmatrix} \in \mathbb{R}^{2 \times 2} \\ &= ab^T X^T\end{aligned}\tag{1372}$$

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

$$\begin{aligned}\nabla_X(Xb) X^T a &= \begin{bmatrix} b_1 & 0 & \\ & b_2 & 0 \\ 0 & b_1 & \\ & 0 & b_2 \end{bmatrix} \begin{bmatrix} X_{11} a_1 + X_{21} a_2 \\ X_{12} a_1 + X_{22} a_2 \end{bmatrix} \in \mathbb{R}^{2 \times 1 \times 2} \\ &= X^T ab^T \in \mathbb{R}^{2 \times 2}\end{aligned}\tag{1373}$$

The solution

$$\nabla_X a^T X^2 b = ab^T X^T + X^T ab^T\tag{1374}$$

can be found from Table D.2.1 or verified using (1367). \square

D.1.2.1 Kronecker product

A partial remedy for venturing into *hyperdimensional* representations, such as the cubix or quartix, is to first vectorize matrices as in (29). This device gives rise to the Kronecker product of matrices \otimes ; **a.k.a**, *direct product* or *tensor product*. Although it sees reversal in the literature, [211, §2.1] we adopt the definition: for $A \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{p \times q}$

$$B \otimes A \triangleq \begin{bmatrix} B_{11}A & B_{12}A & \cdots & B_{1q}A \\ B_{21}A & B_{22}A & \cdots & B_{2q}A \\ \vdots & \vdots & \ddots & \vdots \\ B_{p1}A & B_{p2}A & \cdots & B_{pq}A \end{bmatrix} \in \mathbb{R}^{pm \times qn}\tag{1375}$$

One advantage to vectorization is existence of a traditional two-dimensional matrix representation for the second-order gradient of a real function with respect to a vectorized matrix. For example, from §A.1.1 no.22 (§D.2.1) for square $A, B \in \mathbb{R}^{n \times n}$ [96, §5.2] [10, §3]

$$\nabla_{\text{vec } X}^2 \text{tr}(AXBX^T) = \nabla_{\text{vec } X}^2 \text{vec}(X)^T (B^T \otimes A) \text{vec } X = B \otimes A^T + B^T \otimes A \in \mathbb{R}^{n^2 \times n^2} \quad (1376)$$

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

D.1.3 Chain rules for composite matrix-functions

Given dimensionally compatible matrix-valued functions of matrix variable $f(X)$ and $g(X)$ [137, §15.7]

$$\nabla_X g(f(X)^T) = \nabla_X f^T \nabla_f g \quad (1377)$$

$$\nabla_X^2 g(f(X)^T) = \nabla_X (\nabla_X f^T \nabla_f g) = \nabla_X^2 f \nabla_f g + \nabla_X f^T \nabla_f^2 g \nabla_X f \quad (1378)$$

D.1.3.1 Two arguments

$$\nabla_X g(f(X)^T, h(X)^T) = \nabla_X f^T \nabla_f g + \nabla_X h^T \nabla_h g \quad (1379)$$

D.1.3.1.1 Example. *Chain rule for two arguments.* [28, §1.1]

$$g(f(x)^T, h(x)^T) = (f(x) + h(x))^T A (f(x) + h(x)) \quad (1380)$$

$$f(x) = \begin{bmatrix} x_1 \\ \varepsilon x_2 \end{bmatrix}, \quad h(x) = \begin{bmatrix} \varepsilon x_1 \\ x_2 \end{bmatrix} \quad (1381)$$

$$\nabla_x g(f(x)^T, h(x)^T) = \begin{bmatrix} 1 & 0 \\ 0 & \varepsilon \end{bmatrix} (A + A^T)(f + h) + \begin{bmatrix} \varepsilon & 0 \\ 0 & 1 \end{bmatrix} (A + A^T)(f + h) \quad (1382)$$

$$\nabla_x g(f(x)^T, h(x)^T) = \begin{bmatrix} 1 + \varepsilon & 0 \\ 0 & 1 + \varepsilon \end{bmatrix} (A + A^T) \left(\begin{bmatrix} x_1 \\ \varepsilon x_2 \end{bmatrix} + \begin{bmatrix} \varepsilon x_1 \\ x_2 \end{bmatrix} \right) \quad (1383)$$

$$\lim_{\varepsilon \rightarrow 0} \nabla_x g(f(x)^T, h(x)^T) = (A + A^T)x \quad (1384)$$

from Table [D.2.1](#). \square

These formulae remain correct when the gradients produce hyperdimensional representations:

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 $Y \in \mathbb{R}^{K \times L}$, $\overset{\rightarrow}{dg} \in \mathbb{R}^{M \times N}$ and $\overset{\rightarrow}{dg}^2 \in \mathbb{R}^{M \times N}$ respectively.

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

$$\frac{\partial g_{mn}(X)}{\partial X_{kl}} = \lim_{\Delta t \rightarrow 0} \frac{g_{mn}(X + \Delta t e_k e_l^T) - g_{mn}(X)}{\Delta t} \in \mathbb{R} \quad (1385)$$

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 . The total number of partial derivatives equals $KL MN$ while the gradient is defined in their terms; the mn^{th} entry of the gradient is

$$\nabla g_{mn}(X) = \begin{bmatrix} \frac{\partial g_{mn}(X)}{\partial X_{11}} & \frac{\partial g_{mn}(X)}{\partial X_{12}} & \cdots & \frac{\partial g_{mn}(X)}{\partial X_{1L}} \\ \frac{\partial g_{mn}(X)}{\partial X_{21}} & \frac{\partial g_{mn}(X)}{\partial X_{22}} & \cdots & \frac{\partial g_{mn}(X)}{\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \frac{\partial g_{mn}(X)}{\partial X_{K1}} & \frac{\partial g_{mn}(X)}{\partial X_{K2}} & \cdots & \frac{\partial g_{mn}(X)}{\partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K \times L} \quad (1386)$$

while the gradient is a quartix

$$\nabla g(X) = \begin{bmatrix} \nabla g_{11}(X) & \nabla g_{12}(X) & \cdots & \nabla g_{1N}(X) \\ \nabla g_{21}(X) & \nabla g_{22}(X) & \cdots & \nabla g_{2N}(X) \\ \vdots & \vdots & & \vdots \\ \nabla g_{M1}(X) & \nabla g_{M2}(X) & \cdots & \nabla g_{MN}(X) \end{bmatrix} \in \mathbb{R}^{M \times N \times K \times L} \quad (1387)$$

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

$$\nabla g(X)^{T_1} = \begin{bmatrix} \frac{\partial g(X)}{\partial X_{11}} & \frac{\partial g(X)}{\partial X_{12}} & \cdots & \frac{\partial g(X)}{\partial X_{1L}} \\ \frac{\partial g(X)}{\partial X_{21}} & \frac{\partial g(X)}{\partial X_{22}} & \cdots & \frac{\partial g(X)}{\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \frac{\partial g(X)}{\partial X_{K1}} & \frac{\partial g(X)}{\partial X_{K2}} & \cdots & \frac{\partial g(X)}{\partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K \times L \times M \times N} \quad (1388)$$

When the limit for $\Delta t \in \mathbb{R}$ exists, it is easy to show by substitution of variables in (1385)

$$\frac{\partial g_{mn}(X)}{\partial X_{kl}} Y_{kl} = \lim_{\Delta t \rightarrow 0} \frac{g_{mn}(X + \Delta t Y_{kl} e_k e_l^T) - g_{mn}(X)}{\Delta t} \in \mathbb{R} \quad (1389)$$

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 [137, §15.8]

$$dg_{mn}(X)|_{dX \rightarrow Y} = \sum_{k,l} \frac{\partial g_{mn}(X)}{\partial X_{kl}} Y_{kl} = \text{tr}(\nabla g_{mn}(X)^T Y) \quad (1390)$$

$$= \sum_{k,l} \lim_{\Delta t \rightarrow 0} \frac{g_{mn}(X + \Delta t Y_{kl} e_k e_l^T) - g_{mn}(X)}{\Delta t} \quad (1391)$$

$$= \lim_{\Delta t \rightarrow 0} \frac{g_{mn}(X + \Delta t Y) - g_{mn}(X)}{\Delta t} \quad (1392)$$

$$= \left. \frac{d}{dt} \right|_{t=0} g_{mn}(X + t Y) \quad (1393)$$

where $t \in \mathbb{R}$. Assuming finite Y , equation (1392) is called the *Gâteaux differential* [27, App.A.5] [125, §D.2.1] [234, §5.28] whose existence is implied by the existence of the *Fréchet differential*, the sum in (1390). [157, §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,

$$\begin{aligned}
\vec{\rightarrow Y} dg(X) &\triangleq \left[\begin{array}{cccc} dg_{11}(X) & dg_{12}(X) & \cdots & dg_{1N}(X) \\ dg_{21}(X) & dg_{22}(X) & \cdots & dg_{2N}(X) \\ \vdots & \vdots & & \vdots \\ dg_{M1}(X) & dg_{M2}(X) & \cdots & dg_{MN}(X) \end{array} \right] \bigg|_{dX \rightarrow Y} \in \mathbb{R}^{M \times N} \\
&= \left[\begin{array}{cccc} \text{tr}(\nabla g_{11}(X)^T Y) & \text{tr}(\nabla g_{12}(X)^T Y) & \cdots & \text{tr}(\nabla g_{1N}(X)^T Y) \\ \text{tr}(\nabla g_{21}(X)^T Y) & \text{tr}(\nabla g_{22}(X)^T Y) & \cdots & \text{tr}(\nabla g_{2N}(X)^T Y) \\ \vdots & \vdots & & \vdots \\ \text{tr}(\nabla g_{M1}(X)^T Y) & \text{tr}(\nabla g_{M2}(X)^T Y) & \cdots & \text{tr}(\nabla g_{MN}(X)^T Y) \end{array} \right] \\
&= \left[\begin{array}{cccc} \sum_{k,l} \frac{\partial g_{11}(X)}{\partial X_{kl}} Y_{kl} & \sum_{k,l} \frac{\partial g_{12}(X)}{\partial X_{kl}} Y_{kl} & \cdots & \sum_{k,l} \frac{\partial g_{1N}(X)}{\partial X_{kl}} Y_{kl} \\ \sum_{k,l} \frac{\partial g_{21}(X)}{\partial X_{kl}} Y_{kl} & \sum_{k,l} \frac{\partial g_{22}(X)}{\partial X_{kl}} Y_{kl} & \cdots & \sum_{k,l} \frac{\partial g_{2N}(X)}{\partial X_{kl}} Y_{kl} \\ \vdots & \vdots & & \vdots \\ \sum_{k,l} \frac{\partial g_{M1}(X)}{\partial X_{kl}} Y_{kl} & \sum_{k,l} \frac{\partial g_{M2}(X)}{\partial X_{kl}} Y_{kl} & \cdots & \sum_{k,l} \frac{\partial g_{MN}(X)}{\partial X_{kl}} Y_{kl} \end{array} \right] \quad (1394)
\end{aligned}$$

from which it follows

$$\vec{\rightarrow Y} dg(X) = \sum_{k,l} \frac{\partial g(X)}{\partial X_{kl}} Y_{kl} \quad (1395)$$

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

$$g(X + tY) = g(X) + t \vec{\rightarrow Y} dg(X) + o(t^2) \quad (1396)$$

which is the first-order Taylor series expansion about X . [137, §18.4] [85, §2.3.4] Differentiation with respect to t and subsequent t -zeroing isolates the second term of the expansion. Thus differentiating and zeroing $g(X + tY)$ in t is an operation equivalent to individually differentiating and zeroing every entry $g_{mn}(X + tY)$ as in (1393). So the directional derivative of $g(X)$ in any direction $Y \in \mathbb{R}^{K \times L}$ evaluated at $X \in \text{dom } g$ becomes

$$\vec{\rightarrow Y} dg(X) = \frac{d}{dt} \bigg|_{t=0} g(X + tY) \in \mathbb{R}^{M \times N} \quad (1397)$$

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

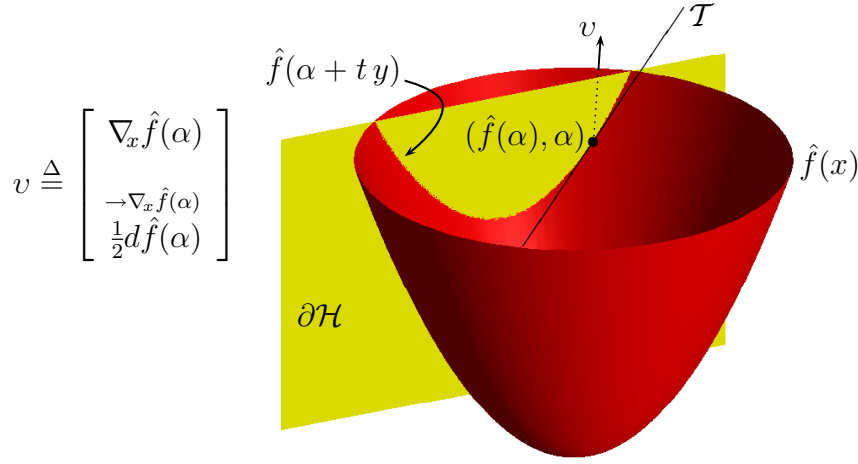


Figure 97: Drawn is a convex quadratic bowl in $\mathbb{R}^2 \times \mathbb{R}$; $\hat{f}(x) = x^T x : \mathbb{R}^2 \rightarrow \mathbb{R}$ versus x on some open disc in \mathbb{R}^2 . Plane slice $\partial\mathcal{H}$ is perpendicular to function domain. Slice intersection with domain connotes bidirectional vector y . Tangent line \mathcal{T} slope at point $(\alpha, \hat{f}(\alpha))$ is directional derivative value $\nabla_x \hat{f}(\alpha)^T y$ (1424) at α in slice direction y . Recall, negative gradient $-\nabla_x \hat{f}(x) \in \mathbb{R}^2$ is always steepest descent direction [248]. [137, §15.6] When vector $v \in \mathbb{R}^3$ entry v_3 is half directional derivative in gradient direction at α and when $\begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = \nabla_x \hat{f}(\alpha)$, then $-v$ points directly toward bowl bottom.

[177, §2.1, §5.4.5] [25, §6.3.1] which is simplest. The derivative with respect to t makes the directional derivative (1397) resemble ordinary calculus (§D.2); *e.g.*, when $g(X)$ is linear, $\overset{\rightarrow Y}{dg}(X) = g(Y)$. [157, §7.2]

D.1.4.1 Interpretation directional derivative

In the case of any differentiable real function $\hat{f}(X) : \mathbb{R}^{K \times L} \rightarrow \mathbb{R}$, the directional derivative of $\hat{f}(X)$ at X in any direction Y yields the slope of \hat{f} along the line $X + tY$ through its domain (parametrized by $t \in \mathbb{R}$) evaluated at $t = 0$. For higher-dimensional functions, by (1394), this slope interpretation can be applied to each entry of the directional derivative. Unlike the gradient, directional derivative does not expand dimension; *e.g.*, directional derivative in (1397) retains the dimensions of g .

Figure 97, for example, shows a plane slice of a real convex bowl-shaped function $\hat{f}(x)$ along a line $\alpha + ty$ through its domain. The slice reveals a one-dimensional real function of t ; $\hat{f}(\alpha + ty)$. The directional derivative at $x = \alpha$ in direction y is the slope of $\hat{f}(\alpha + ty)$ 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. (1424) 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 §3.1.1.4)

D.1.4.1.1 Theorem. *Directional derivative condition for optimization.* [157, §7.4] Suppose $\hat{f}(X) : \mathbb{R}^{K \times L} \rightarrow \mathbb{R}$ is minimized on convex set $\mathcal{C} \subseteq \mathbb{R}^{p \times k}$ by X^* , and the directional derivative of \hat{f} exists there. Then for all $X \in \mathcal{C}$

$$\begin{matrix} \rightarrow X - X^* \\ d\hat{f}(X) \geq 0 \end{matrix} \quad (1398)$$

◇

D.1.4.1.2 Example. *Simple bowl.*

Bowl function (Figure 97)

$$\hat{f}(x) : \mathbb{R}^K \rightarrow \mathbb{R} \triangleq (x - a)^T(x - a) - b \quad (1399)$$

has function offset $-b \in \mathbb{R}$, axis of revolution at $x = a$, and positive definite Hessian (1355) everywhere in its domain (an open *hyperdisc* in \mathbb{R}^K); *id est*, strictly convex quadratic $\hat{f}(x)$ has unique global minimum equal to $-b$ at $x = a$. A vector $-v$ based anywhere in $\text{dom } \hat{f} \times \mathbb{R}$ pointing toward the unique bowl-bottom is specified:

$$v \propto \begin{bmatrix} x - a \\ \hat{f}(x) + b \end{bmatrix} \in \mathbb{R}^K \times \mathbb{R} \quad (1400)$$

Such a vector is

$$v = \begin{bmatrix} \nabla_x \hat{f}(x) \\ -\nabla_x \hat{f}(x) \\ \frac{1}{2} d\hat{f}(x) \end{bmatrix} \quad (1401)$$

since the gradient is

$$\nabla_x \hat{f}(x) = 2(x - a) \quad (1402)$$

and the directional derivative in the direction of the gradient is (1424)

$$\begin{aligned} \xrightarrow{\nabla_x \hat{f}(x)} \\ d\hat{f}(x) = \nabla_x \hat{f}(x)^T \nabla_x \hat{f}(x) = 4(x - a)^T (x - a) = 4(\hat{f}(x) + b) \end{aligned} \quad (1403)$$

□

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,

$$\nabla \frac{\partial g_{mn}(X)}{\partial X_{kl}} = \frac{\partial \nabla g_{mn}(X)}{\partial X_{kl}} = \begin{bmatrix} \frac{\partial^2 g_{mn}(X)}{\partial X_{kl} \partial X_{11}} & \frac{\partial^2 g_{mn}(X)}{\partial X_{kl} \partial X_{12}} & \cdots & \frac{\partial^2 g_{mn}(X)}{\partial X_{kl} \partial X_{1L}} \\ \frac{\partial^2 g_{mn}(X)}{\partial X_{kl} \partial X_{21}} & \frac{\partial^2 g_{mn}(X)}{\partial X_{kl} \partial X_{22}} & \cdots & \frac{\partial^2 g_{mn}(X)}{\partial X_{kl} \partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \frac{\partial^2 g_{mn}(X)}{\partial X_{kl} \partial X_{K1}} & \frac{\partial^2 g_{mn}(X)}{\partial X_{kl} \partial X_{K2}} & \cdots & \frac{\partial^2 g_{mn}(X)}{\partial X_{kl} \partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K \times L} \quad (1404)$$

$$\begin{aligned} \nabla^2 g_{mn}(X) &= \begin{bmatrix} \nabla \frac{\partial g_{mn}(X)}{\partial X_{11}} & \nabla \frac{\partial g_{mn}(X)}{\partial X_{12}} & \cdots & \nabla \frac{\partial g_{mn}(X)}{\partial X_{1L}} \\ \nabla \frac{\partial g_{mn}(X)}{\partial X_{21}} & \nabla \frac{\partial g_{mn}(X)}{\partial X_{22}} & \cdots & \nabla \frac{\partial g_{mn}(X)}{\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \nabla \frac{\partial g_{mn}(X)}{\partial X_{K1}} & \nabla \frac{\partial g_{mn}(X)}{\partial X_{K2}} & \cdots & \nabla \frac{\partial g_{mn}(X)}{\partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K \times L \times K \times L} \\ &= \begin{bmatrix} \frac{\partial \nabla g_{mn}(X)}{\partial X_{11}} & \frac{\partial \nabla g_{mn}(X)}{\partial X_{12}} & \cdots & \frac{\partial \nabla g_{mn}(X)}{\partial X_{1L}} \\ \frac{\partial \nabla g_{mn}(X)}{\partial X_{21}} & \frac{\partial \nabla g_{mn}(X)}{\partial X_{22}} & \cdots & \frac{\partial \nabla g_{mn}(X)}{\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \frac{\partial \nabla g_{mn}(X)}{\partial X_{K1}} & \frac{\partial \nabla g_{mn}(X)}{\partial X_{K2}} & \cdots & \frac{\partial \nabla g_{mn}(X)}{\partial X_{KL}} \end{bmatrix} \end{aligned} \quad (1405)$$

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

$$\nabla^2 g(X) = \begin{bmatrix} \nabla^2 g_{11}(X) & \nabla^2 g_{12}(X) & \cdots & \nabla^2 g_{1N}(X) \\ \nabla^2 g_{21}(X) & \nabla^2 g_{22}(X) & \cdots & \nabla^2 g_{2N}(X) \\ \vdots & \vdots & & \vdots \\ \nabla^2 g_{M1}(X) & \nabla^2 g_{M2}(X) & \cdots & \nabla^2 g_{MN}(X) \end{bmatrix} \in \mathbb{R}^{M \times N \times K \times L \times K \times L} \quad (1406)$$

$$\nabla^2 g(X)^{T_1} = \begin{bmatrix} \nabla \frac{\partial g(X)}{\partial X_{11}} & \nabla \frac{\partial g(X)}{\partial X_{12}} & \dots & \nabla \frac{\partial g(X)}{\partial X_{1L}} \\ \nabla \frac{\partial g(X)}{\partial X_{21}} & \nabla \frac{\partial g(X)}{\partial X_{22}} & \dots & \nabla \frac{\partial g(X)}{\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \nabla \frac{\partial g(X)}{\partial X_{K1}} & \nabla \frac{\partial g(X)}{\partial X_{K2}} & \dots & \nabla \frac{\partial g(X)}{\partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K \times L \times M \times N \times K \times L} \quad (1407)$$

$$\nabla^2 g(X)^{T_2} = \begin{bmatrix} \frac{\partial \nabla g(X)}{\partial X_{11}} & \frac{\partial \nabla g(X)}{\partial X_{12}} & \dots & \frac{\partial \nabla g(X)}{\partial X_{1L}} \\ \frac{\partial \nabla g(X)}{\partial X_{21}} & \frac{\partial \nabla g(X)}{\partial X_{22}} & \dots & \frac{\partial \nabla g(X)}{\partial X_{2L}} \\ \vdots & \vdots & & \vdots \\ \frac{\partial \nabla g(X)}{\partial X_{K1}} & \frac{\partial \nabla g(X)}{\partial X_{K2}} & \dots & \frac{\partial \nabla g(X)}{\partial X_{KL}} \end{bmatrix} \in \mathbb{R}^{K \times L \times K \times L \times M \times N} \quad (1408)$$

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

$$\frac{\partial^2 g_{mn}(X)}{\partial X_{kl} \partial X_{ij}} = \lim_{\Delta \tau, \Delta t \rightarrow 0} \frac{g_{mn}(X + \Delta t e_k e_l^T + \Delta \tau e_i e_j^T) - g_{mn}(X + \Delta t e_k e_l^T) - (g_{mn}(X + \Delta \tau e_i e_j^T) - g_{mn}(X))}{\Delta \tau \Delta t} \quad (1409)$$

Differentiating (1389) and then scaling by Y_{ij}

$$\begin{aligned} \frac{\partial^2 g_{mn}(X)}{\partial X_{kl} \partial X_{ij}} Y_{kl} Y_{ij} &= \lim_{\Delta t \rightarrow 0} \frac{\partial g_{mn}(X + \Delta t Y_{kl} e_k e_l^T) - \partial g_{mn}(X)}{\partial X_{ij} \Delta t} Y_{ij} \\ &= \lim_{\Delta \tau, \Delta t \rightarrow 0} \frac{g_{mn}(X + \Delta t Y_{kl} e_k e_l^T + \Delta \tau Y_{ij} e_i e_j^T) - g_{mn}(X + \Delta t Y_{kl} e_k e_l^T) - (g_{mn}(X + \Delta \tau Y_{ij} e_i e_j^T) - g_{mn}(X))}{\Delta \tau \Delta t} \end{aligned} \quad (1410)$$

which can be proved by substitution of variables in (1409). The mn^{th} second-order total differential due to any $Y \in \mathbb{R}^{K \times L}$ is

$$d^2 g_{mn}(X)|_{dX \rightarrow Y} = \sum_{i,j} \sum_{k,l} \frac{\partial^2 g_{mn}(X)}{\partial X_{kl} \partial X_{ij}} Y_{kl} Y_{ij} = \text{tr} \left(\nabla_X \text{tr}(\nabla g_{mn}(X)^T Y)^T Y \right) \quad (1411)$$

$$= \sum_{i,j} \lim_{\Delta t \rightarrow 0} \frac{\partial g_{mn}(X + \Delta t Y) - \partial g_{mn}(X)}{\partial X_{ij} \Delta t} Y_{ij} \quad (1412)$$

$$= \lim_{\Delta t \rightarrow 0} \frac{g_{mn}(X + 2\Delta t Y) - 2g_{mn}(X + \Delta t Y) + g_{mn}(X)}{\Delta t^2} \quad (1413)$$

$$= \left. \frac{d^2}{dt^2} \right|_{t=0} g_{mn}(X + t Y) \quad (1414)$$

Hence the second directional derivative,

$$\begin{aligned}
\stackrel{\rightarrow}{dg}^2(X) &\triangleq \left[\begin{array}{cccc} d^2g_{11}(X) & d^2g_{12}(X) & \cdots & d^2g_{1N}(X) \\ d^2g_{21}(X) & d^2g_{22}(X) & \cdots & d^2g_{2N}(X) \\ \vdots & \vdots & & \vdots \\ d^2g_{M1}(X) & d^2g_{M2}(X) & \cdots & d^2g_{MN}(X) \end{array} \right] \bigg|_{dX \rightarrow Y} \in \mathbb{R}^{M \times N} \\
&= \left[\begin{array}{cccc} \text{tr}(\nabla \text{tr}(\nabla g_{11}(X)^T Y)^T Y) & \text{tr}(\nabla \text{tr}(\nabla g_{12}(X)^T Y)^T Y) & \cdots & \text{tr}(\nabla \text{tr}(\nabla g_{1N}(X)^T Y)^T Y) \\ \text{tr}(\nabla \text{tr}(\nabla g_{21}(X)^T Y)^T Y) & \text{tr}(\nabla \text{tr}(\nabla g_{22}(X)^T Y)^T Y) & \cdots & \text{tr}(\nabla \text{tr}(\nabla g_{2N}(X)^T Y)^T Y) \\ \vdots & \vdots & & \vdots \\ \text{tr}(\nabla \text{tr}(\nabla g_{M1}(X)^T Y)^T Y) & \text{tr}(\nabla \text{tr}(\nabla g_{M2}(X)^T Y)^T Y) & \cdots & \text{tr}(\nabla \text{tr}(\nabla g_{MN}(X)^T Y)^T Y) \end{array} \right] \\
&= \left[\begin{array}{cccc} \sum_{i,j} \sum_{k,l} \frac{\partial^2 g_{11}(X)}{\partial X_{kl} \partial X_{ij}} Y_{kl} Y_{ij} & \sum_{i,j} \sum_{k,l} \frac{\partial^2 g_{12}(X)}{\partial X_{kl} \partial X_{ij}} Y_{kl} Y_{ij} & \cdots & \sum_{i,j} \sum_{k,l} \frac{\partial^2 g_{1N}(X)}{\partial X_{kl} \partial X_{ij}} Y_{kl} Y_{ij} \\ \sum_{i,j} \sum_{k,l} \frac{\partial^2 g_{21}(X)}{\partial X_{kl} \partial X_{ij}} Y_{kl} Y_{ij} & \sum_{i,j} \sum_{k,l} \frac{\partial^2 g_{22}(X)}{\partial X_{kl} \partial X_{ij}} Y_{kl} Y_{ij} & \cdots & \sum_{i,j} \sum_{k,l} \frac{\partial^2 g_{2N}(X)}{\partial X_{kl} \partial X_{ij}} Y_{kl} Y_{ij} \\ \vdots & \vdots & & \vdots \\ \sum_{i,j} \sum_{k,l} \frac{\partial^2 g_{M1}(X)}{\partial X_{kl} \partial X_{ij}} Y_{kl} Y_{ij} & \sum_{i,j} \sum_{k,l} \frac{\partial^2 g_{M2}(X)}{\partial X_{kl} \partial X_{ij}} Y_{kl} Y_{ij} & \cdots & \sum_{i,j} \sum_{k,l} \frac{\partial^2 g_{MN}(X)}{\partial X_{kl} \partial X_{ij}} Y_{kl} Y_{ij} \end{array} \right] \\
&\quad (1415)
\end{aligned}$$

from which it follows

$$\stackrel{\rightarrow}{dg}^2(X) = \sum_{i,j} \sum_{k,l} \frac{\partial^2 g(X)}{\partial X_{kl} \partial X_{ij}} Y_{kl} Y_{ij} = \sum_{i,j} \frac{\partial}{\partial X_{ij}} \stackrel{\rightarrow}{dg}(X) Y_{ij} \quad (1416)$$

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

$$g(X + tY) = g(X) + t \stackrel{\rightarrow}{dg}(X) + \frac{1}{2!} t^2 \stackrel{\rightarrow}{dg}^2(X) + o(t^3) \quad (1417)$$

which is the second-order Taylor series expansion about X . [137, §18.4] [85, §2.3.4] Differentiating twice with respect to t and subsequent t -zeroing isolates the third term of the expansion. Thus differentiating and zeroing $g(X + tY)$ in t is an operation equivalent to individually differentiating and zeroing every entry $g_{mn}(X + tY)$ as in (1414). So the second directional derivative becomes

$$\stackrel{\rightarrow}{dg}^2(X) = \frac{d^2}{dt^2} \bigg|_{t=0} g(X + tY) \in \mathbb{R}^{M \times N} \quad (1418)$$

[177, §2.1, §5.4.5] [25, §6.3.1] which is again simplest. (confer (1397))

D.1.6 Taylor series

Series expansions of the differentiable matrix-valued function $g(X)$, of matrix argument, were given earlier in (1396) and (1417). Assuming $g(X)$ has continuous first-, second-, and third-order gradients over the open set $\text{dom } g$, then for $X \in \text{dom } g$ and any $Y \in \mathbb{R}^{K \times L}$ the complete Taylor series on some open interval of $\mu \in \mathbb{R}$ is expressed

$$g(X + \mu Y) = g(X) + \mu \vec{d}g(X) + \frac{1}{2!} \mu^2 \vec{d}g^2(X) + \frac{1}{3!} \mu^3 \vec{d}g^3(X) + o(\mu^4) \quad (1419)$$

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

$$g(Y) = g(X) + \vec{d}g(X) + \frac{1}{2!} \vec{d}g^2(X) + \frac{1}{3!} \vec{d}g^3(X) + o(\|Y\|^4) \quad (1420)$$

which are third-order expansions about X . The *mean value theorem* from calculus is what insures the finite order of the series. [28, §1.1] [27, App.A.5] [125, §0.4] [137]

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

$$\vec{d}g(X) = \text{tr}(\nabla g(X)^T Y) \quad (1421)$$

$$\vec{d}g^2(X) = \text{tr}\left(\nabla_X \text{tr}(\nabla g(X)^T Y)^T Y\right) = \text{tr}\left(\nabla_X \vec{d}g(X)^T Y\right) \quad (1422)$$

$$\vec{d}g^3(X) = \text{tr}\left(\nabla_X \text{tr}\left(\nabla_X \text{tr}(\nabla g(X)^T Y)^T Y\right)^T Y\right) = \text{tr}\left(\nabla_X \vec{d}g^2(X)^T Y\right) \quad (1423)$$

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

$$\vec{d}g(X) = \nabla g(X)^T Y \quad (1424)$$

$$\vec{d}g^2(X) = Y^T \nabla^2 g(X) Y \quad (1425)$$

$$\vec{d}g^3(X) = \nabla_X (Y^T \nabla^2 g(X) Y)^T Y \quad (1426)$$

and so on.

D.1.6.0.1 Exercise. *log det.* (confer [39, p.644])
Find the first two terms of the Taylor series expansion (1420) for $\log \det X$.

▼

D.1.7 Correspondence of gradient to derivative

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

D.1.7.1 first-order

Removing from (1397) the evaluation at $t = 0$, ^{D.3} we find an expression for the directional derivative of $g(X)$ in direction Y evaluated anywhere along a line $X + tY$ (parametrized by t) intersecting $\text{dom } g$

$$\vec{\rightarrow}^Y dg(X + tY) = \frac{d}{dt}g(X + tY) \quad (1427)$$

In the general case $g(X) : \mathbb{R}^{K \times L} \rightarrow \mathbb{R}^{M \times N}$, from (1390) and (1393) we find

$$\text{tr}(\nabla_X g_{mn}(X + tY)^T Y) = \frac{d}{dt}g_{mn}(X + tY) \quad (1428)$$

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 (1421) we have simply

$$\text{tr}(\nabla_X g(X + tY)^T Y) = \frac{d}{dt}g(X + tY) \quad (1429)$$

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

$$\nabla_X g(X + tY)^T Y = \frac{d}{dt}g(X + tY) \quad (1430)$$

^{D.3}Justified by replacing X with $X + tY$ in (1390)-(1392); beginning,

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

D.1.7.1.1 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,

$$\text{tr}(\nabla_X g(X + tY)^T Y) = \text{tr}(2ww^T(X^T + tY^T)Y) \quad (1431)$$

$$= 2w^T(X^T Y + tY^T Y)w \quad (1432)$$

Applying the equivalence (1429),

$$\frac{d}{dt}g(X + tY) = \frac{d}{dt}w^T(X + tY)^T(X + tY)w \quad (1433)$$

$$= w^T(X^T Y + Y^T X + 2tY^T Y)w \quad (1434)$$

$$= 2w^T(X^T Y + tY^T Y)w \quad (1435)$$

which is the same as (1432); hence, equivalence is demonstrated.

It is easy to extract $\nabla g(X)$ from (1435) knowing only (1429):

$$\begin{aligned} \text{tr}(\nabla_X g(X + tY)^T Y) &= 2w^T(X^T Y + tY^T Y)w \\ &= 2\text{tr}(ww^T(X^T + tY^T)Y) \\ \text{tr}(\nabla_X g(X)^T Y) &= 2\text{tr}(ww^T X^T Y) \\ &\Leftrightarrow \\ \nabla_X g(X) &= 2Xww^T \end{aligned} \quad (1436)$$

□

D.1.7.2 second-order

Likewise removing the evaluation at $t=0$ from (1418),

$$\overset{\rightarrow Y}{dg^2}(X + tY) = \frac{d^2}{dt^2}g(X + tY) \quad (1437)$$

we can find a similar relationship between the second-order gradient and the second derivative: In the general case $g(X) : \mathbb{R}^{K \times L} \rightarrow \mathbb{R}^{M \times N}$ from (1411) and (1414),

$$\text{tr}\left(\nabla_X \text{tr}(\nabla_X g_{mn}(X + tY)^T Y)^T Y\right) = \frac{d^2}{dt^2}g_{mn}(X + tY) \quad (1438)$$

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

$$\text{tr}\left(\nabla_X \text{tr}(\nabla_X g(X + tY)^T Y)^T Y\right) = \frac{d^2}{dt^2}g(X + tY) \quad (1439)$$

From (1425), the simpler case, where the real function $g(X) : \mathbb{R}^K \rightarrow \mathbb{R}$ has vector argument,

$$Y^T \nabla_X^2 g(X + tY) Y = \frac{d^2}{dt^2} g(X + tY) \quad (1440)$$

D.1.7.2.1 Example. *Second-order gradient.*

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

$$h(X) \triangleq \nabla g(X) = X^{-1} \in \text{int } \mathbb{S}_+^K \quad (1441)$$

so $\nabla^2 g(X) = \nabla h(X)$. By (1428) and (1396), for $Y \in \mathbb{S}^K$

$$\text{tr}(\nabla h_{mn}(X)^T Y) = \left. \frac{d}{dt} \right|_{t=0} h_{mn}(X + tY) \quad (1442)$$

$$= \left(\left. \frac{d}{dt} \right|_{t=0} h(X + tY) \right)_{mn} \quad (1443)$$

$$= \left(\left. \frac{d}{dt} \right|_{t=0} (X + tY)^{-1} \right)_{mn} \quad (1444)$$

$$= -(X^{-1} Y X^{-1})_{mn} \quad (1445)$$

Setting Y to a member of the standard basis $E_{kl} = e_k e_l^T$, for $k, l \in \{1 \dots K\}$, and employing a property of the trace function (31) we find

$$\nabla^2 g(X)_{mnkl} = \text{tr}(\nabla h_{mn}(X)^T E_{kl}) = \nabla h_{mn}(X)_{kl} = -(X^{-1} E_{kl} X^{-1})_{mn} \quad (1446)$$

$$\nabla^2 g(X)_{kl} = \nabla h(X)_{kl} = -(X^{-1} E_{kl} X^{-1}) \in \mathbb{R}^{K \times K} \quad (1447)$$

□

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 the differentiation.

D.2 Tables of gradients and derivatives

[96] [43]

- When proving results for symmetric matrices algebraically, it is critical to take gradients ignoring symmetry and to then substitute symmetric entries afterward.
- $a, b \in \mathbb{R}^n$, $x, y \in \mathbb{R}^k$, $A, B \in \mathbb{R}^{m \times n}$, $X, Y \in \mathbb{R}^{K \times L}$, $t, \mu \in \mathbb{R}$, $i, j, k, \ell, K, L, m, n, M, N$ are integers, unless otherwise noted.
- x^μ means $\delta(\delta(x)^\mu)$ for $\mu \in \mathbb{R}$; *id est*, entrywise vector exponentiation. δ is the main-diagonal linear operator (1036). $x^0 \triangleq \mathbf{1}$, $X^0 \triangleq I$ 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), $\log x$, $\operatorname{sgn} x$, $\sin x$, x/y (Hadamard quotient), \sqrt{x} (entrywise square root), *etcetera*, are maps $f : \mathbb{R}^k \rightarrow \mathbb{R}^k$ that maintain dimension; *e.g.*, (§A.1.1)

$$\frac{d}{dx} x^{-1} \triangleq \nabla_x \mathbf{1}^T \delta(x)^{-1} \mathbf{1} \quad (1448)$$

- The standard basis: $\{E_{kl} = e_k e_\ell^T \in \mathbb{R}^{K \times K} \mid k, \ell \in \{1 \dots K\}\}$
- For A a scalar or matrix, we have the Taylor series [45, §3.6]

$$e^A = \sum_{k=0}^{\infty} \frac{1}{k!} A^k \quad (1449)$$

Further, [215, §5.4]

$$e^A \succ 0 \quad \forall A \in \mathbb{S}^m \quad (1450)$$

- For all square A and integer k

$$\det^k A = \det A^k \quad (1451)$$

- Table entries with notation $X \in \mathbb{R}^{2 \times 2}$ have been algebraically verified in that dimension but may hold more broadly.

D.2.1 Algebraic

$\nabla_x x = \nabla_x x^T = I \in \mathbb{R}^{k \times k}$	$\nabla_X X = \nabla_X X^T \triangleq I \in \mathbb{R}^{K \times L \times K \times L}$ (identity)
$\nabla_x (Ax - b) = A^T$	
$\nabla_x (x^T A - b^T) = A$	
$\nabla_x (Ax - b)^T (Ax - b) = 2A^T (Ax - b)$	
$\nabla_x^2 (Ax - b)^T (Ax - b) = 2A^T A$	
$\nabla_x (x^T Ax + 2x^T By + y^T Cy) = (A + A^T)x + 2By$	
$\nabla_x^2 (x^T Ax + 2x^T By + y^T Cy) = A + A^T$	
	$\nabla_X a^T X b = \nabla_X b^T X^T a = ab^T$
	$\nabla_X a^T X^2 b = X^T ab^T + ab^T X^T$
	$\nabla_X a^T X^{-1} b = -X^{-T} ab^T X^{-T}$
	$\nabla_X (X^{-1})_{kl} = \frac{\partial X^{-1}}{\partial X_{kl}} = -X^{-1} E_{kl} X^{-1}, \text{ confer } (1388)(1447)$
$\nabla_x a^T x^T x b = 2xa^T b$	$\nabla_X a^T X^T X b = X(ab^T + ba^T)$
$\nabla_x a^T x x^T b = (ab^T + ba^T)x$	$\nabla_X a^T X X^T b = (ab^T + ba^T)X$
$\nabla_x a^T x^T x a = 2xa^T a$	$\nabla_X a^T X^T X a = 2Xaa^T$
$\nabla_x a^T x x^T a = 2aa^T x$	$\nabla_X a^T X X^T a = 2aa^T X$
$\nabla_x a^T y x^T b = ba^T y$	$\nabla_X a^T Y X^T b = ba^T Y$
$\nabla_x a^T y^T x b = yb^T a$	$\nabla_X a^T Y^T X b = Yab^T$
$\nabla_x a^T x y^T b = ab^T y$	$\nabla_X a^T X Y^T b = ab^T Y$
$\nabla_x a^T x^T y b = ya^T b$	$\nabla_X a^T X^T Y b = Yba^T$

Algebraic continued

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

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

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

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

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

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

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

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

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

D.2.2 Trace Kronecker

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

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

D.2.3 Trace

$\nabla_x \mu x = \mu I$	$\nabla_X \operatorname{tr} \mu X = \nabla_X \mu \operatorname{tr} X = \mu I$
$\nabla_x \mathbf{1}^T \delta(x)^{-1} \mathbf{1} = \frac{d}{dx} x^{-1} = -x^{-2}$	$\nabla_X \operatorname{tr} X^{-1} = -X^{-2T}$
$\nabla_x \mathbf{1}^T \delta(x)^{-1} y = -\delta(x)^{-2} y$	$\nabla_X \operatorname{tr}(X^{-1} Y) = \nabla_X \operatorname{tr}(Y X^{-1}) = -X^{-T} Y^T X^{-T}$
$\frac{d}{dx} x^\mu = \mu x^{\mu-1}$	$\nabla_X \operatorname{tr} X^\mu = \mu X^{(\mu-1)T}, \quad X \in \mathbb{R}^{2 \times 2}$
	$\nabla_X \operatorname{tr} X^j = j X^{(j-1)T}$
$\nabla_x (b - a^T x)^{-1} = (b - a^T x)^{-2} a$	$\nabla_X \operatorname{tr}((B - AX)^{-1}) = ((B - AX)^{-2} A)^T$
$\nabla_x (b - a^T x)^\mu = -\mu (b - a^T x)^{\mu-1} a$	
$\nabla_x x^T y = \nabla_x y^T x = y$	$\nabla_X \operatorname{tr}(X^T Y) = \nabla_X \operatorname{tr}(Y X^T) = \nabla_X \operatorname{tr}(Y^T X) = \nabla_X \operatorname{tr}(X Y^T) = Y$
	$\nabla_X \operatorname{tr}(A X B X^T) = \nabla_X \operatorname{tr}(X B X^T A) = A^T X B^T + A X B$
	$\nabla_X \operatorname{tr}(A X B X) = \nabla_X \operatorname{tr}(X B X A) = A^T X^T B^T + B^T X^T A^T$
	$\nabla_X \operatorname{tr}(A X A X A X) = \nabla_X \operatorname{tr}(X A X A X A) = 3(A X A X A)^T$
	$\nabla_X \operatorname{tr}(Y X^k) = \nabla_X \operatorname{tr}(X^k Y) = \sum_{i=0}^{k-1} (X^i Y X^{k-1-i})^T$
	$\nabla_X \operatorname{tr}(Y^T X X^T Y) = \nabla_X \operatorname{tr}(X^T Y Y^T X) = 2 Y Y^T X$
	$\nabla_X \operatorname{tr}(Y^T X^T X Y) = \nabla_X \operatorname{tr}(X Y Y^T X^T) = 2 X Y Y^T$
	$\nabla_X \operatorname{tr}((X + Y)^T (X + Y)) = 2(X + Y)$
	$\nabla_X \operatorname{tr}((X + Y)(X + Y)) = 2(X + Y)^T$
	$\nabla_X \operatorname{tr}(A^T X B) = \nabla_X \operatorname{tr}(X^T A B^T) = A B^T$
	$\nabla_X \operatorname{tr}(A^T X^{-1} B) = \nabla_X \operatorname{tr}(X^{-T} A B^T) = -X^{-T} A B^T X^{-T}$
	$\nabla_X a^T X b = \nabla_X \operatorname{tr}(b a^T X) = \nabla_X \operatorname{tr}(X b a^T) = a b^T$
	$\nabla_X b^T X^T a = \nabla_X \operatorname{tr}(X^T a b^T) = \nabla_X \operatorname{tr}(a b^T X^T) = a b^T$
	$\nabla_X a^T X^{-1} b = \nabla_X \operatorname{tr}(X^{-T} a b^T) = -X^{-T} a b^T X^{-T}$
	$\nabla_X a^T X^\mu b = \dots$

Trace continued

$$\begin{aligned}
\frac{d}{dt} \operatorname{tr} g(X+tY) &= \operatorname{tr} \frac{d}{dt} g(X+tY) \\
\frac{d}{dt} \operatorname{tr}(X+tY) &= \operatorname{tr} Y \\
\frac{d}{dt} \operatorname{tr}^j(X+tY) &= j \operatorname{tr}^{j-1}(X+tY) \operatorname{tr} Y \\
\frac{d}{dt} \operatorname{tr}(X+tY)^j &= j \operatorname{tr}((X+tY)^{j-1} Y) \quad (\forall j) \\
\frac{d}{dt} \operatorname{tr}((X+tY)Y) &= \operatorname{tr} Y^2 \\
\frac{d}{dt} \operatorname{tr}((X+tY)^k Y) &= \frac{d}{dt} \operatorname{tr}(Y(X+tY)^k) = k \operatorname{tr}((X+tY)^{k-1} Y^2), \quad k \in \{0, 1, 2\} \\
\frac{d}{dt} \operatorname{tr}((X+tY)^k Y) &= \frac{d}{dt} \operatorname{tr}(Y(X+tY)^k) = \operatorname{tr} \sum_{i=0}^{k-1} (X+tY)^i Y (X+tY)^{k-1-i} Y \\
\frac{d}{dt} \operatorname{tr}((X+tY)^{-1} Y) &= -\operatorname{tr}((X+tY)^{-1} Y (X+tY)^{-1} Y) \\
\frac{d}{dt} \operatorname{tr}(B^T(X+tY)^{-1} A) &= -\operatorname{tr}(B^T(X+tY)^{-1} Y (X+tY)^{-1} A) \\
\frac{d}{dt} \operatorname{tr}(B^T(X+tY)^{-T} A) &= -\operatorname{tr}(B^T(X+tY)^{-T} Y^T (X+tY)^{-T} A) \\
\frac{d}{dt} \operatorname{tr}(B^T(X+tY)^{-k} A) &= \dots, \quad k > 0 \\
\frac{d}{dt} \operatorname{tr}(B^T(X+tY)^\mu A) &= \dots, \quad -1 \leq \mu \leq 1, \quad X, Y \in \mathbb{S}_+^M \\
\frac{d^2}{dt^2} \operatorname{tr}(B^T(X+tY)^{-1} A) &= 2 \operatorname{tr}(B^T(X+tY)^{-1} Y (X+tY)^{-1} Y (X+tY)^{-1} A) \\
\frac{d}{dt} \operatorname{tr}((X+tY)^T A (X+tY)) &= \operatorname{tr}(Y^T A X + X^T A Y + 2t Y^T A Y) \\
\frac{d^2}{dt^2} \operatorname{tr}((X+tY)^T A (X+tY)) &= 2 \operatorname{tr}(Y^T A Y) \\
\frac{d}{dt} \operatorname{tr}((X+tY) A (X+tY)) &= \operatorname{tr}(Y A X + X A Y + 2t Y A Y) \\
\frac{d^2}{dt^2} \operatorname{tr}((X+tY) A (X+tY)) &= 2 \operatorname{tr}(Y A Y)
\end{aligned}$$

D.2.4 Log 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.

$\frac{d}{dx} \log x = x^{-1}$	$\nabla_X \log \det X = X^{-T}$
$\frac{d}{dx} \log x^{-1} = -x^{-1}$	$\nabla_X^2 \log \det(X)_{kl} = \frac{\partial X^{-T}}{\partial X_{kl}} = -(X^{-1} E_{kl} X^{-1})^T, \quad \text{confer (1405)(1447)}$
$\frac{d}{dx} \log x^\mu = \mu x^{-1}$	$\nabla_X \log \det X^{-1} = -X^{-T}$
	$\nabla_X \log \det^\mu X = \mu X^{-T}$
	$\nabla_X \log \det X^\mu = \mu X^{-T}, \quad X \in \mathbb{R}^{2 \times 2}$
	$\nabla_X \log \det X^k = \nabla_X \log \det^k X = k X^{-T}$
	$\nabla_X \log \det^\mu(X + tY) = \mu(X + tY)^{-T}$
$\nabla_x \log(a^T x + b) = a \frac{1}{a^T x + b}$	$\nabla_X \log \det(AX + B) = A^T(AX + B)^{-T}$
	$\nabla_X \log \det(I \pm A^T X A) = \dots$
	$\nabla_X \log \det(X + tY)^k = \nabla_X \log \det^k(X + tY) = k(X + tY)^{-T}$
	$\frac{d}{dt} \log \det(X + tY) = \text{tr}((X + tY)^{-1} Y)$
	$\frac{d^2}{dt^2} \log \det(X + tY) = -\text{tr}((X + tY)^{-1} Y (X + tY)^{-1} Y)$
	$\frac{d}{dt} \log \det(X + tY)^{-1} = -\text{tr}((X + tY)^{-1} Y)$
	$\frac{d^2}{dt^2} \log \det(X + tY)^{-1} = \text{tr}((X + tY)^{-1} Y (X + tY)^{-1} Y)$
	$\frac{d}{dt} \log \det(\delta(A(x + ty) + a)^2 + \mu I)$ $= \text{tr}((\delta(A(x + ty) + a)^2 + \mu I)^{-1} 2\delta(A(x + ty) + a)\delta(Ay))$

D.2.5 Determinant

$$\nabla_X \det X = \nabla_X \det X^T = \det(X) X^{-T}$$

$$\nabla_X \det X^{-1} = -\det(X^{-1}) X^{-T} = -\det(X)^{-1} X^{-T}$$

$$\nabla_X \det^\mu X = \mu \det^\mu(X) X^{-T}$$

$$\nabla_X \det X^\mu = \mu \det(X^\mu) X^{-T}, \quad X \in \mathbb{R}^{2 \times 2}$$

$$\nabla_X \det X^k = k \det^{k-1}(X) (\operatorname{tr}(X) I - X^T), \quad X \in \mathbb{R}^{2 \times 2}$$

$$\nabla_X \det X^k = \nabla_X \det^k X = k \det(X^k) X^{-T} = k \det^k(X) X^{-T}$$

$$\nabla_X \det^\mu(X + tY) = \mu \det^\mu(X + tY) (X + tY)^{-T}$$

$$\nabla_X \det(X + tY)^k = \nabla_X \det^k(X + tY) = k \det^k(X + tY) (X + tY)^{-T}$$

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

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

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

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

$$\frac{d}{dt} \det^\mu(X + tY) = \dots$$

D.2.6 Logarithmic

$$\frac{d}{dt} \log(X + tY)^\mu = \dots, \quad -1 \leq \mu \leq 1, \quad X, Y \in \mathbb{S}_+^M \quad [128, \S 6.6, \text{prob.20}]$$

D.2.7 Exponential

[45, §3.6, §4.5] [215, §5.4]

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

$$\nabla_X \text{tr} e^{YX} = e^{Y^T X^T} Y^T = Y^T e^{X^T Y^T}$$

log-sum-exp & geometric mean [39, p.74]...

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

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

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

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

e^X for symmetric X of dimension less than 3 [39, pg.110]...