Operations Research
04. Optimization Fundamentals

The Chain Rule

Definition (The Jacobian)**.** Let V be open in $\mathbb{R}^n$, $\mathbf{x} \in V$, and $g_i : V \to \mathbb{R}$, $i = 1, 2, \ldots, m$ be C^1 on V. The Jacobian of $\mathbf{g}(\mathbf{x}) : \mathbb{R}^n \to \mathbb{R}^m$ is defined as

$$\mathrm{D}\,\mathbf{g}(\mathbf{x}) = \begin{pmatrix} \frac{\partial g_1}{\partial x_1} & \frac{\partial g_1}{\partial x_2} & \cdots & \frac{\partial g_1}{\partial x_n} \\ \frac{\partial g_2}{\partial x_1} & \frac{\partial g_2}{\partial x_2} & \cdots & \frac{\partial g_2}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial g_m}{\partial x_1} & \frac{\partial g_m}{\partial x_2} & \cdots & \frac{\partial g_m}{\partial x_n} \end{pmatrix} (\mathbf{x})$$

Theorem (Rudin (1976) 9.15; Apostol (1974) Theorem 12.7; Wade (2009) 11.28)**.** Suppose that $\mathbf{f}$ and $\mathbf{g}$ are vector functions. If $\mathbf{g}$ is differentiable at $\mathbf{a}$ and $\mathbf{f}$ is differentiable at $\mathbf{g}(\mathbf{a})$, then $\mathbf{f} \circ \mathbf{g}$ is differentiable at $\mathbf{a}$ and

$$\mathrm{D}(\mathbf{f} \circ \mathbf{g})(\mathbf{a}) = \mathrm{D}\,\mathbf{f}(\mathbf{g}(\mathbf{a}))\ \mathrm{D}\,\mathbf{g}(\mathbf{a})$$

More explicitly, if f is a differentiable function of $x_1, x_2, \ldots, x_n$, and each x_j is a differentiable function of $t_1, t_2, \ldots, t_m$, $n, m \geqslant 1$; then f is a differentiable function of $t_1, t_2, \ldots, t_m$ with

$$\frac{\partial f}{\partial t_i} = \frac{\partial f}{\partial x_1}\frac{\partial x_1}{\partial t_i} + \frac{\partial f}{\partial x_2}\frac{\partial x_2}{\partial t_i} + \cdots + \frac{\partial f}{\partial x_n}\frac{\partial x_n}{\partial t_i}$$

Example. Let $w = f(xz, yz)$, where f is a differentiable function. Prove that $x\dfrac{\partial w}{\partial x} + y\dfrac{\partial w}{\partial y} = z\dfrac{\partial w}{\partial z}$.

Solution. Write $u(x,y,z) = xz$ and $v(x,y,z) = yz$ so that $w(x,y,z) = f(u(x,y,z), v(x,y,z))$. By the chain rule,

$$\frac{\partial w}{\partial x}(x,y,z) = \frac{\partial}{\partial x}\left[f(u(x,y,z), v(x,y,z))\right]$$
$$= \frac{\partial f}{\partial u}(u(x,y,z), v(x,y,z))\frac{\partial u}{\partial x}(x,y,z) + \frac{\partial f}{\partial v}(u(x,y,z), v(x,y,z))\frac{\partial v}{\partial x}(x,y,z)$$
$$= z\frac{\partial f}{\partial u}(xz, yz)$$

$$\frac{\partial w}{\partial y}(x,y,z) = \frac{\partial}{\partial y}\left[f(u(x,y,z), v(x,y,z))\right]$$
$$= \frac{\partial f}{\partial u}(u(x,y,z), v(x,y,z))\frac{\partial u}{\partial y}(x,y,z) + \frac{\partial f}{\partial v}(u(x,y,z), v(x,y,z))\frac{\partial v}{\partial y}(x,y,z)$$
$$= z\frac{\partial f}{\partial v}(xz, yz)$$

$$
\begin{aligned}
&\frac{\partial w}{\partial z}(x,y,z) = \frac{\partial}{\partial z}\big[f(u(x,y,z),v(x,y,z))\big] \\
&= \frac{\partial f}{\partial u}\big(u(x,y,z),v(x,y,z)\big)\frac{\partial u}{\partial z}(x,y,z) + \frac{\partial f}{\partial v}\big(u(x,y,z),v(x,y,z)\big)\frac{\partial v}{\partial z}(x,y,z) \\
&= x\frac{\partial f}{\partial u}(xz,yz) + y\frac{\partial f}{\partial v}(xz,yz)
\end{aligned}
$$

So

$$
\begin{aligned}
\frac{\partial w}{\partial x} + y\frac{\partial w}{\partial y} &= xz\frac{\partial f}{\partial u}(xz,yz) + yz\frac{\partial f}{\partial v}(xz,yz) \\
&= z\left[x\frac{\partial f}{\partial u}(xz,yz) + y\frac{\partial f}{\partial v}(xz,yz)\right] = z\frac{\partial w}{\partial z}
\end{aligned}
$$

Unconstrained Optimization Problems

Theorem (Rudin (1976) 4.16; Apostol (1974) Theorem 4.27; Wade (2009) 9.57)**.** Given $S \subseteq \mathbb{R}^n$ and continuous $f : S \to \mathbb{R}$; if S is compact, then

$$M = \sup\{f(\mathbf{x}) : \mathbf{x} \in S\} \quad \text{and} \quad m = \inf\{f(\mathbf{x}) : \mathbf{x} \in S\}$$

are finite real numbers. Moreover, there exists points $\mathbf{x}_\mathrm{M}$, $\mathbf{x}_\mathrm{m} \in S$ such that $M = f(\mathbf{x}_\mathrm{M})$ and $m = f(\mathbf{x}_\mathrm{m})$.

Definition. Given $S \subseteq \mathbb{R}^n$, $f : S \to \mathbb{R}$ and $B(\mathbf{x}, h) \equiv \{\mathbf{y} \in \mathbb{R}^n \mid |\mathbf{y} - \mathbf{x}| < h\}$, f achieves

- global maximum $f(\mathbf{x}_\mathrm{M})$ at $\mathbf{x}_\mathrm{M} \in S$: $f(\mathbf{x}_\mathrm{M}) \geqslant f(\mathbf{x})$, $\forall\, \mathbf{x} \in S$.
- global minimum $f(\mathbf{x}_\mathrm{m})$ at $\mathbf{x}_\mathrm{m} \in S$: $f(\mathbf{x}_\mathrm{m}) \leqslant f(\mathbf{x})$, $\forall\, \mathbf{x} \in S$.
- local maximum $f(\mathbf{x}_0)$ at $\mathbf{x}_0 \in S$: $\exists\, h_0 > 0$ s.t. $f(\mathbf{x}_0) \geqslant f(\mathbf{x})$, $\forall\, \mathbf{x} \in B(\mathbf{x}_0, h_0) \cap S$.
- local minimum $f(\mathbf{x}_1)$ at $\mathbf{x}_1 \in S$: $\exists\, h_1 > 0$ s.t. $f(\mathbf{x}_1) \leqslant f(\mathbf{x})$, $\forall\, \mathbf{x} \in B(\mathbf{x}_1, h_1) \cap S$.

Theorem (necessary conditions for extremum)**.** Given $S \subseteq \mathbb{R}^n$ and differentiable $f : S \to \mathbb{R}$, if f achieves extremum at an interior $\mathbf{c} \in S$, then $\nabla f(\mathbf{c}) = \mathbf{0}$.

Proof. If $\mathbf{c} = (c_1, c_2, \ldots, c_n)$, let

$$g_j(t) \equiv f(c_1, c_2, \ldots, c_{j-1}, t, c_{j+1}, \ldots, c_n), \quad j = 1, 2, \ldots, n$$

For f achieves extremum at $\mathbf{c}$, $f(\mathbf{c}) = g_j(c_j)$, g_j achieves extremum at $c_j \implies g_j'(t)\Big|_{t=c_j} = 0 \implies D_j f(\mathbf{c}) = 0 \; \forall\, j$, so $\nabla f(\mathbf{c}) = \mathbf{0}$.

Theorem. Given $S \subseteq \mathbb{R}^n$, if $f : S \to \mathbb{R}$ achieves extremum at $\mathbf{c} \in S$, then $\mathbf{c}$ can possibly be a

- critical point: $\nabla f(\mathbf{c}) = \mathbf{0}$.
- singular point: f is non-differentiable at $\mathbf{c}$.
- boundary point of S.

Definition (Hessian Matrix)**.** Given $S \subseteq \mathbb{R}^n$, an interior point $\mathbf{c}$ of S, and a differentiable function $f : S \to \mathbb{R}$,

$$\mathbf{H}(f, \mathbf{c}) = \begin{pmatrix} f_{11} & f_{12} & \cdots & f_{1n} \\ f_{21} & f_{22} & \cdots & f_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ f_{n1} & f_{n2} & \cdots & f_{nn} \end{pmatrix}, \quad f_{ij} = \frac{\partial^2 f}{\partial x_j \partial x_i}(\mathbf{c}), \quad i,\, j = 1,\, 2,\, \ldots,\, n.$$

Definition (Matrix Positive/Negative Definiteness)**.** Given an $n \times n$ real symmetric matrix $\mathbf{A}$. For any $\mathbf{v} \in \mathbb{R}^n \neq \mathbf{0}$, $\mathbf{A}$ is

- positive-definite: $\mathbf{vAv}^\top > 0$
- negative-definite: $\mathbf{vAv}^\top < 0$
- positive-semidefinite: $\mathbf{vAv}^\top \geqslant 0$
- negative-semidefinite: $\mathbf{vAv}^\top \leqslant 0$

Definition (Minor)**.** Given an $n \times n$ matrix $\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix}$

and minor $\mathbf{A}\begin{pmatrix} i_1,\, i_2,\, \cdots,\, i_k \\ j_1,\, j_2,\, \cdots,\, j_k \end{pmatrix} = \begin{vmatrix} a_{i_1 j_1} & a_{i_1 j_2} & \cdots & a_{i_1 j_k} \\ a_{i_2 j_1} & a_{i_2 j_2} & \cdots & a_{i_2 j_k} \\ \vdots & \vdots & \ddots & \vdots \\ a_{i_k j_1} & a_{i_k j_2} & \cdots & a_{i_k j_k} \end{vmatrix}$, $1 \leqslant k \leqslant n$, $1 \leqslant i_1 < i_2 < \cdots < i_k \leqslant n$, $1 \leqslant j_1 < j_2 < \cdots < j_k \leqslant n$.

- $\Delta_k \equiv \mathbf{A}\begin{pmatrix} i_1,\, i_2,\, \cdots,\, i_k \\ i_1,\, i_2,\, \cdots,\, i_k \end{pmatrix}$ is the k-th order principal minor of A.

- $M_k \equiv \mathbf{A}\begin{pmatrix} 1,\, 2,\, \cdots,\, k \\ 1,\, 2,\, \cdots,\, k \end{pmatrix}$ is the k-th order leading principal minor of A.

Theorem (Criteria for Matrix Positive/Negative Definiteness)**.** Given an $n \times n$ real symmetric matrix $\mathbf{A}$, then $\forall\, k \leqslant n$, $\mathbf{A}$ is

- positive-definite $\iff M_k > 0$

- negative-definite $\iff (-1)^k M_k > 0$

- positive-semidefinite $\iff \Delta_k \geqslant 0$

- negative-semidefinite $\iff (-1)^k \Delta_k \geqslant 0$

Example. Consider the matrix $\mathbf{A} = \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix}$: Let $\mathbf{v} = \langle a, b, c \rangle$, $\mathbf{vAv}^\top = \begin{pmatrix} a & b & c \end{pmatrix} \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} 2a-b & -a+2b-c & -b+2c \end{pmatrix} \cdot \begin{pmatrix} a \\ b \\ c \end{pmatrix} = (2a-b)a + (-a+2b-c)b + (-b+2c)c = 2a^2 - 2ab + 2b^2 - 2bc + 2c^2 = a^2 + (a-b)^2 + (b-c)^2 + c^2 > 0$, except when $a = b = c = 0$, so it is positive-definite. Also, $\mathbf{A}$'s M_1, M_2, M_3 are 2, $\begin{vmatrix} 2 & -1 \\ -1 & 2 \end{vmatrix} = 3$, $\begin{vmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{vmatrix} = 4$ respectively, by the above criteria $\mathbf{A}$ is positive-definite.

Theorem (Second Derivative Test)**.** Given $S \subseteq \mathbb{R}^n$ and a differentiable function $f : S \to \mathbb{R}$, and f at an interior point $\mathbf{c}$ of S has $\nabla f(\mathbf{c}) = 0$. If $\mathbf{H}(f, \mathbf{c})$ is

- positive-definite $\implies$ f has a local minimum at $\mathbf{c}$.
- negative-definite $\implies$ f has a local maximum at $\mathbf{c}$.

Fact. Given $S \subseteq \mathbb{R}^2$ and a differentiable function $f : S \to \mathbb{R}$, and f at an interior point (a, b) of S has $\nabla f(a, b) = 0$. Let

$$D = f_{xx}(a, b) \cdot f_{yy}(a, b) - (f_{xy}(a, b))^2$$

- If $D > 0$ and $f_{xx}(a, b) > 0$, then f has a local minimum at (a, b).
- If $D > 0$ and $f_{xx}(a, b) < 0$, then f has a local maximum at (a, b).
- If $D < 0$, then (a, b) is a saddle point.

Example. Find the critical points of $f(x,y) = x^3 + xy^2 - 3x^2 - 4y^2 + 4$ and classify them.

Solution. From $f_x(x,y) = 3x^2 + y^2 - 6x$, $f_y(x,y) = 2xy - 8y$, the critical points are (x,y) that simultaneously satisfy these two equations being zero. Therefore $\{3x^2 + y^2 - 6x = 0\} \wedge \{y\,(x-4) = 0\} \implies \{y = 0 \wedge 3x^2 - 6x = 0\} \vee \{x = 4 \wedge 3 \cdot 4^2 + y^2 + 6 \cdot 4 = 0\}$, So the critical points are $(0,0)$, $(2,0)$. Also $f_{xx} = 6x - 6$, $f_{yy} = 2x - 8$, $f_{xy} = f_{yx} = 2y$, classified as follows:

Critical Point	$f_{xx}f_{yy} - f_{xy}^2$	f_{xx}	Classification
$(0,0)$	$(-6) \times (-8) - (0)^2 > 0$	-6	Local maximum
$(2,0)$	$6 \times (-4) - 0^2 < 0$		Saddle point

Example. Find the critical points of $f(x,y) = xy\,(5x+y-15)$ and classify them.

Solution. From $f_x(x,y) = y\,(5x+y-15)+xy\,(5) = y\,(5x+y-15)+y\,(5x) = y\,(10x+y-15)$, $f_y(x,y) = x\,(5x+y-15)+xy\,(1) = x\,(5x+y-15)+x\,(y) = x\,(5x+2y-15)$, the critical points are (x,y) that simultaneously satisfy these two equations being zero. Therefore $\{y=0 \;\vee\; 10x+y-15=0\} \;\wedge\; \{x=0 \;\vee\; 5x+2y-15=0\} \implies \{y=0 \;\wedge\; x=0\} \;\vee\; \{y=0 \;\wedge\; 5x+2y=15\} \;\vee\; \{10x+y=15 \;\wedge\; x=0\} \;\vee\; \{10x+y=15 \;\wedge\; 5x+2y=15\}$, So the critical points are $(0,0)$, $(3,0)$, $(0,15)$, $(1,5)$. Also $f_{xx} = 10y$, $f_{yy} = 2x$, $f_{xy} = f_{yx} = 10x+2y-15$, classified as follows:

Critical Point	$f_{xx}f_{yy} - f_{xy}^2$	f_{xx}	Classification
$(0,0)$	$0 \times 0 - (-15)^2 < 0$		Saddle point
$(3,0)$	$0 \times 6 - 15^2 < 0$		Saddle point
$(0,15)$	$150 \times 0 - 15^2 < 0$		Saddle point
$(1,5)$	$50 \times 2 - 5^2 > 0$	50	Local minimum

Example. Find the maximum and the minimum of $f(x,y) = (x+y)\,e^{-x^2-y^2}$ on $S : x^2+y^2 \leqslant 1$.

Solution. Since f is differentiable, it has no singular points; the extrema of f occur at critical points ($\mathbf{c} \in S$, $\nabla f(\mathbf{c}) = 0$) and boundary points of S.

- From $f_x = e^{-x^2-y^2} + (x+y)\,e^{-x^2-y^2}\,(-2x) = (-2x^2 - 2xy + 1)\,e^{-x^2-y^2}$, $f_y = e^{-x^2-y^2} + (x+y)\,e^{-x^2-y^2}\,(-2y) = (-2y^2 - 2xy + 1)\,e^{-x^2-y^2}$, the critical points (x,y) satisfy $2x^2+2xy = 1$ and $2y^2+2xy = 1$, which gives $(x,y) = \left(\frac{1}{2}, \frac{1}{2}\right)$, $\left(-\frac{1}{2}, -\frac{1}{2}\right)$.
- Boundary points $x^2+y^2 = 1$: Let $x = \cos t$, $y = \sin t$, $0 \leqslant t \leqslant 2\pi$, then $f(x,y)$ becomes $g(t) \equiv (\cos t + \sin t)\,e^{-1}$; $g'(t) = (-\sin t + \cos t)\,e^{-1} = 0$ solves to $t = \frac{\pi}{4}, \frac{5\pi}{4}$; also consider boundary $t = 0, 2\pi$, i.e., $(x,y) = \left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right)$, $\left(-\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}\right)$, $(1,0)$.

Candidate Point	$f(x,y)$	Classification
$\left(\frac{1}{2}, \frac{1}{2}\right)$	$e^{-\frac{1}{2}}$	Maximum
$\left(-\frac{1}{2}, -\frac{1}{2}\right)$	$-e^{-\frac{1}{2}}$	Minimum
$\left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right)$	$\sqrt{2}\,e^{-1}$	
$\left(-\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}\right)$	$-\sqrt{2}\,e^{-1}$	
$(1,0)$	e^{-1}	

Example. Find the maximum and the minimum of $f(x, y) = x^3 + xy^2 - 3x^2 - 4y^2 + 4$ on $S : x^2 + y^2 \leqslant 1$.

Solution. Since f is differentiable, it has no singular points; the extrema of f occur at critical points ($\mathbf{c} \in S$, $\nabla f(\mathbf{c}) = 0$) and boundary points of S ($x^2 + y^2 = 1$).

- From $f_x = 3x^2 + y^2 - 6x$, $f_y = 2xy - 8y$, the critical points (x, y) satisfy $3x^2 + y^2 - 6x = 0$ and $2xy - 8y = 0$, which gives $(x, y) = (0, 0),\ (2, 0)$; $(2, 0)$ is outside S and not applicable.

- Boundary points $x^2 + y^2 = 1$: Substitute $y^2 = 1 - x^2$ then $f(x, y)$ becomes $g(x) = x^3 + x\left(1 - x^2\right) - 3x^2 - 4\left(1 - x^2\right) + 4 = x + x^2$, $-1 \leqslant x \leqslant 1$; $g'(x) = 1 + 2x = 0$ solves to $x = -\frac{1}{2}$, i.e., the extrema of $g(x)$ occur at $x = \pm 1$ and $-\frac{1}{2} \implies (x, y) = (-\frac{1}{2}, \pm\frac{\sqrt{3}}{2}),\ (1, 0),\ (-1, 0)$.

Candidate Point	$f(x, y)$	Classification
$(0, 0)$	4	Maximum
$\left(-\frac{1}{2}, \pm\frac{\sqrt{3}}{2}\right)$	$-\frac{1}{4}$	Minimum
$(1, 0)$	2	
$(-1, 0)$	0	

Example. Find the maximum and the minimum of $f(x,y) = xy - x^3y^2$ on $S: 0 \leqslant x \leqslant 1,\ 0 \leqslant y \leqslant 1$.

Solution. Since f is differentiable, it has no singular points; the extrema of f occur at critical points ($\mathbf{c} \in S$, $\nabla f(\mathbf{c}) = 0$) and boundary points of S.

- From $f_x = y - 3x^2y^2$, $f_y = x - 2x^3y$, the critical points (x,y) satisfy $y - 3x^2y^2 = y\,(1 - 3x^2y) = 0$ and $x - 2x^3y = x\,(1 - 2x^2y) = 0$, so $y = 0 \ \vee \ 1 - 3x^2y = 0$ and $x = 0 \ \vee \ 1 - 2x^2y = 0$; which gives $(x,y) = (0,0)$.

- The boundary points consist of $L_1 :\ x = 0 \ \wedge \ 0 \leqslant y \leqslant 1$, $L_2 :\ y = 0 \ \wedge \ 0 \leqslant x \leqslant 1$, $L_3 :\ x = 1 \ \wedge \ 0 \leqslant y \leqslant 1$, $L_4 :\ y = 1 \ \wedge \ 0 \leqslant x \leqslant 1$.

  - L_1: $f(x,y) = 0$.
  - L_2: $f(x,y) = 0$.
  - L_3: $x = 1$, $0 \leqslant y \leqslant 1$, $f(x,y)$ becomes $g(y) = y - y^2$, $g'(y) = 1 - 2y = 0$ solves to $y = \frac{1}{2}$, i.e., the extrema of $g(y)$ occur at $y = 0,\ 1,\ \frac{1}{2} \implies (x,y) = (1,0),\ (1,1),\ (1,\frac{1}{2})$
  - L_4: $y = 1$, $0 \leqslant x \leqslant 1$, $f(x,y)$ becomes $h(x) = x - x^3$, $h'(x) = 1 - 3x^2 = 0$ solves to $x = \pm\frac{1}{\sqrt{3}}$ (negative not applicable), i.e., the

extrema of $h(x)$ occur at $x = 0,\ 1,\ \frac{1}{\sqrt{3}} \implies (x, y) = (0, 1),\ (1, 1),\ (\frac{1}{\sqrt{3}}, 1)$.

Candidate Point	$f(x, y)$	Classification
$(0, 0 \leqslant y \leqslant 1)$	0	Minimum
$(0 \leqslant x \leqslant 1, 0)$	0	Minimum
$(0, 0)$	0	Minimum
$(1, 0)$	0	Minimum
$(1, 1)$	0	Minimum
$(1, \frac{1}{2})$	$\frac{1}{4}$	
$(0, 1)$	0	Minimum
$(\frac{1}{\sqrt{3}}, 1)$	$\frac{2}{3\sqrt{3}}$	Maximum

Example. Find the maximum and the minimum of $f(x, y) = xy + 2x + y$ in the triangular region S formed by $(0, 0)$, $(1, 0)$, $(0, 2)$.

Solution. Since f is differentiable, it has no singular points; the extrema of f occur at critical points ($\mathbf{c} \in S$, $\nabla f(\mathbf{c}) = 0$) and boundary points of S.

- From $f_x = y + 2$, $f_y = x + 1$, the critical points (x, y) satisfy $y + 2 = 0$ and $x + 1 = 0$, so $(x, y) = (-1, -2)$.
- The boundary points consist of $L_1 : \ x = 0 \ \wedge \ 0 \leqslant y \leqslant 2$, $L_2 : \ y = 0 \ \wedge \ 0 \leqslant x \leqslant 1$, $L_3 : \ (1, 0) — (0, 2)$.
  - L_1: $(x, y) = (0, 0)$, $(0, 2)$.
  - L_2: $(x, y) = (0, 0)$, $(1, 0)$.
  - L_3: $y = -2x + 2$, $0 \leqslant x \leqslant 1$, $f(x, y)$ becomes $g(x) = x\,(-2x + 2) + 2x + (-2x + 2) = -2x^2 + 2x + 2$, $g'(x) = -4x + 2 = 0$ solves to $x = \frac{1}{2}$, i.e., the extrema of $g(x)$ occur at $x = 0,\ 1,\ \frac{1}{2}$ $\Longrightarrow$ $(x, y) = (0, 2)$, $(1, 0)$, $\left(\frac{1}{2}, 1\right)$

Candidate Point	$f(x, y)$	Classification
$(0, 0)$	0	Minimum
$(0, 2)$	2	
$(1, 0)$	2	
$\left(\frac{1}{2}, 1\right)$	$\frac{5}{2}$	Maximum

Example. Find the maximum and the minimum of $f(x,y) = xy\,e^{-\frac{x^2+y^2}{2}}$ on $S:\ \{(x,y)\,|\,x^2+y^2 \leqslant 4,\ x \geqslant 0,\ y \geqslant 0\}$.

Solution. Since f is differentiable, it has no singular points; the extrema of f occur at critical points ($\mathbf{c} \in S$, $\nabla f(\mathbf{c}) = 0$) and boundary points of S.

- From $f_x(x,y) = y\,e^{-\frac{x^2+y^2}{2}} + xy\,e^{-\frac{x^2+y^2}{2}}\,(-x) = y(1-x^2)\,e^{-\frac{x^2+y^2}{2}}$, $f_y(x,y) = x\,e^{-\frac{x^2+y^2}{2}} + xy\,e^{-\frac{x^2+y^2}{2}}\,(-y) = x(1-y^2)\,e^{-\frac{x^2+y^2}{2}}$, the critical points (x,y) satisfy $y\,(1-x^2) = 0$ and $x\,(1-y^2) = 0$, which gives $(x,y) = (0,0)$, $(1,1)$, $(1,-1)$, $(-1,1)$, $(-1,-1)$; only $(0,0)$, $(1,1)$ are inside S.
- The boundary points consist of $L_1:\ x = 0 \wedge 0 \leqslant y \leqslant 2$, $L_2:\ y = 0 \wedge 0 \leqslant x \leqslant 2$, $L_3:\ x^2+y^2 = 4$ in the first quadrant.
  - L_1: $f(x,y) = 0$.
  - L_2: $f(x,y) = 0$.
  - L_3: Let $x = 2\cos t$, $y = 2\sin t$, $0 \leqslant t \leqslant \frac{\pi}{2}$, then $f(x,y)$ becomes $g(t) \equiv 4\cos t\sin t\,e^{-2}$; $g'(t) = \cos 2t\,4e^{-2} = 0$ solves to $t = \frac{\pi}{4}$; also consider boundary $t = 0,\ \frac{\pi}{2}$, i.e., $(x,y) = (\sqrt{2},\sqrt{2}),\ (2,0),\ (0,2)$.

Candidate Point	$f(x,y)$	Classification
$(0,0)$	0	Minimum
$(1,1)$	e^{-1}	Maximum
$(0, 0 \leqslant y \leqslant 2)$	0	Minimum
$(0 \leqslant x \leqslant 2, 0)$	0	Minimum
$(\sqrt{2}, \sqrt{2})$	$2e^{-2}$	
$(2,0)$	0	Minimum
$(0,2)$	0	Minimum

Equalities Constrained Optimization Problems: The Lagrange Multipliers Method

Theorem (Apostol (1974) Theorem 13.12; Wade (2009) 11.63)**.** Given an open set $S \subseteq \mathbb{R}^n$, differentiable functions $f : S \to \mathbb{R}$ and $g_j : S \to \mathbb{R}$, $j = 1, 2, \ldots, m$, $m < n$, and $X_0 = \{\mathbf{x} \in S \mid g_j(\mathbf{x}) = 0,\, j = 1, 2, \ldots, m\}$. If f has an extremum at $\mathbf{x}_0 \in S \cap X_0$ and $\det\left(D_i g_j(\mathbf{x}_0)\right) \neq 0$, then

$$\exists\, \lambda_1, \lambda_2, \ldots, \lambda_m \quad \text{s.t.} \quad D_i f(\mathbf{x}_0) + \sum_{j=1}^{m} \lambda_j D_i g_j(\mathbf{x}_0) = 0, \quad i = 1, 2, \ldots, n$$

Remark. Let $\mathcal{L} \equiv f + \sum_{j=1}^{m} \lambda_j\, g_j$, the sufficient condition can be rewritten as

$$\begin{aligned} D_i\, \mathcal{L}(\mathbf{x}_0) &= 0, \quad i = 1, 2, \ldots, n \\ g_j(\mathbf{x}_0) &= 0, \quad j = 1, 2, \ldots, m \end{aligned}$$

Example. Find the maximum and minimum values of $x^2 - 10x - y^2$ on $x^2 + 4y^2 = 16$.

Solution. Let $\mathcal{L} = x^2 - 10x - y^2 + \lambda\,(x^2 + 4y^2 - 16)$, then

$$\frac{\partial \mathcal{L}}{\partial x} = 2x - 10 + 2\lambda x = 0 \implies x - 5 + \lambda x = 0 \tag{1}$$

$$\frac{\partial \mathcal{L}}{\partial y} = -2y + 8\lambda y = 0 \implies -y + 4\lambda y = 0 \tag{2}$$

$$x^2 + 4y^2 - 16 = 0 \tag{3}$$

From (2) $(1 - 4\lambda)y = 0$, so $y = 0 \ \vee \ \lambda = \frac{1}{4}$. If $y = 0$, from (3) $x = \pm 4$; if $\lambda = \frac{1}{4}$, from (1) $(1 + \lambda)\,x = 5 \implies x = 4$, substituting into (3) gives $y = 0$. Therefore, the extremum points are $(x, y) = (4, 0)$, $(-4, 0)$; $x^2 - 10x - y^2$ has a maximum value of 56 (at $(x, y) = (-4, 0)$), and a minimum value of -24 (at $(x, y) = (4, 0)$).

Example. Find the point on $x^2 = y^2 + z^2$ that is closest to $(0, 1, 3)$.

Solution. The square of the distance is $x^2 + (y-1)^2 + (z-3)^2$, with the constraint $x^2 - y^2 - z^2 = 0$. Let $\mathcal{L} = x^2 + (y-1)^2 + (z-3)^2 + \lambda(x^2 - y^2 - z^2)$, then

$$\frac{\partial \mathcal{L}}{\partial x} = 2x + 2\lambda x = 0 \implies (1+\lambda)x = 0 \tag{4}$$

$$\frac{\partial \mathcal{L}}{\partial y} = 2\,(y-1) - 2\lambda y = 0 \implies (1-\lambda)y = 1 \tag{5}$$

$$\frac{\partial \mathcal{L}}{\partial z} = 2\,(z-3) - 2\lambda z = 0 \implies (1-\lambda)z = 3 \tag{6}$$

$$x^2 - y^2 - z^2 = 0 \tag{7}$$

From (4) $(1+\lambda)x = 0$, so $x = 0 \ \vee \ \lambda = -1$. If $x = 0$, from (7) $y = z = 0$; if $\lambda = -1$, from (5) $y = \frac{1}{2}$, from (6) $z = \frac{3}{2}$, substituting into (7) gives $x = \pm\sqrt{\frac{5}{2}}$. Therefore, the extremum points are $(x, y, z) = (0, 0, 0)$, $\left(\pm\sqrt{\frac{5}{2}}, \frac{1}{2}, \frac{3}{2}\right)$; the minimum value of the square of the distance $x^2 + (y-1)^2 + (z-3)^2$ is 5, occurring at $(x, y, z) = \left(\pm\sqrt{\frac{5}{2}}, \frac{1}{2}, \frac{3}{2}\right)$.

Example. Find the maximum and minimum values of $f(x, y, z) = (x+z)\, e^y$ on $x^2 + y^2 + z^2 = 6$.

Solution. Let $\mathcal{L} = (x + z)\, e^y + \lambda\, (x^2 + y^2 + z^2 - 6)$, then

$$\frac{\partial \mathcal{L}}{\partial x} = e^y + 2\lambda x = 0 \tag{8}$$

$$\frac{\partial \mathcal{L}}{\partial y} = (x + z)\, e^y + 2\lambda y = 0 \tag{9}$$

$$\frac{\partial \mathcal{L}}{\partial z} = e^y + 2\lambda z = 0 \tag{10}$$

$$x^2 + y^2 + z^2 - 6 = 0 \tag{11}$$

From (8), (10) $2\,\lambda(x - z) = 0$, so $\lambda = 0 \;\vee\; x = z$. If $\lambda = 0$, then from (8) $e^y = 0$ which is impossible, so $x = z$. From (8) $e^y = -2\lambda x$, substituting into (9) $2x\,(-2\lambda x) + 2\lambda y = 0 \implies y = 2x^2$, substituting into (11) gives $x^2 + 4x^4 + x^2 = 6 \implies (4x^2 + 6)(x^2 - 1) = 0 \implies x = \pm 1$. Therefore, the extremum points are $(x, y, z) = (1, 2, 1)$, $(-1, 2, -1)$; $(x + z)\, e^y$ has a maximum value of $2e^2$ (at $(x, y, z) = (1, 2, 1)$), and a minimum value of $-2e^2$ (at $(x, y, z) = (-1, 2, -1)$).

Example. If L is the curve of intersection of $z^2 = x^2 + y^2$ and $x - 2z = 3$, find the point on L that is closest to the origin and the shortest distance.

Solution. The objective is $x^2 + y^2 + z^2$ with constraints $x^2 + y^2 - z^2 = 0$ and $x - 2z - 3 = 0$. Let $\mathcal{L} = x^2 + y^2 + z^2 + \lambda_1 (x^2 + y^2 - z^2) + \lambda_2 (x - 2z - 3)$, then

$$\frac{\partial \mathcal{L}}{\partial x} = 2x + 2\lambda_1 x + \lambda_2 = 0 \implies 2(1 + \lambda_1)x + \lambda_2 = 0 \tag{12}$$

$$\frac{\partial \mathcal{L}}{\partial y} = 2y + 2\lambda_1 y = 0 \implies (1 + \lambda_1)y = 0 \tag{13}$$

$$\frac{\partial \mathcal{L}}{\partial z} = 2z - 2\lambda_1 z - 2\lambda_2 = 0 \implies (1 - \lambda_1)z - \lambda_2 = 0 \tag{14}$$

$$x^2 + y^2 - z^2 = 0 \tag{15}$$

$$x - 2z - 3 = 0 \tag{16}$$

From (13) $(1 + \lambda_1)y = 0$, so $y = 0 \ \vee \ \lambda_1 = -1$. If $y = 0$, from (15) $x^2 = z^2 \implies x = \pm z$. If $x = z$, from (16) $x = z = -3$. If $x = -z$, from (16) $x = 1$, $z = -1$; if $\lambda_1 = -1$, from (12) $\lambda_2 = 0$, from (14) $z = 0$, substituting into (15) gives $x = y = 0$, which contradicts (16). Therefore, the extremum points are $(x, y, z) = (-3, 0, -3)$, $(1, 0, -1)$; the minimum value of the square of the distance $x^2 + y^2 + z^2$ is 2 (shortest distance is $\sqrt{2}$), occurring at $(x, y, z) = (1, 0, -1)$.

Descent Direction Iteration

Starting with a design point $\mathbf{x}^{(1)}$ and generate a sequence of points $\{\mathbf{x}^{(k)}\}$ to converge to a local minimum:

- Check whether $\mathbf{x}^{(k)}$ satisfies the termination conditions. If it does, terminate; otherwise proceed to the next step.
- Determine the *descent direction* $\mathbf{d}^{(k)}$ using local info such as the gradient or Hessian.
- Determine the *step size* or *learning rate* $\alpha^{(k)}$.
- Compute the next point $\mathbf{x}^{(k+1)}$ according to

$$\mathbf{x}^{(k+1)} \longleftarrow \mathbf{x}^{(k)} + \alpha^{(k)}\,\mathbf{d}^{(k)}$$

Each optimization methods has its own way of determining $\mathbf{d}$ and α.

First Order Method

- $\mathbf{g}^{(k)} = \nabla f(\mathbf{x}^{(k)})$, $\mathbf{d}^{(k)} = -\dfrac{\mathbf{g}^{(k)}}{\|\mathbf{g}^{(k)}\|}$
- $\alpha^{(k)} = \underset{\alpha}{\operatorname{argmin}}\ f(\mathbf{x}^{(k)} + \alpha\,\mathbf{d}^{(k)})$
- The above optimization implies the directional derivative equals zero, i.e.

$$\nabla f(\mathbf{x}^{(k)} + \alpha\,\mathbf{d}^{(k)})^\top\,\mathbf{d}^{(k)} = 0$$

- We know that

$$\mathbf{d}^{(k+1)} = -\frac{\nabla f(\mathbf{x}^{(k)} + \alpha\,\mathbf{d}^{(k)})}{\|\nabla f(\mathbf{x}^{(k)} + \alpha\,\mathbf{d}^{(k)})\|}$$

Hence ${\mathbf{d}^{(k+1)}}^\top\,\mathbf{d}^{(k)} = 0$.

Second Order Method

Recall Newton's method of finding the root of $f(x) = 0$.

- Given initial x_0
- Update by $x_{n+1} = x_n - \dfrac{f(x_n)}{f'(x_n)}$; $n = 0, 1, 2, ...$

Apply to $f(x) = x^2 - a$, we have the `Python` code:

```
def mysqrt(a):
    x = a
    for i in range(100):
        x -= (x ** 2 - a) / (2 * x)
    return x
```

- To find the optimal value of $f(x)$, we are actually finding the critical points: the root of $f'(x) = 0$. So
  - Given initial x_0
  - Update by $x_{n+1} = x_n - \dfrac{f'(x_n)}{f''(x_n)}$; $n = 0, 1, 2, ...$
- Another viewpoint: the univariate second order Taylor expansion of $f(x)$ w.r.t. x_n is

$$f(x) \approx q(x) = f(x_n) + f'(x_n)(x - x_n) + \frac{1}{2} f''(x_n)(x - x_n)^2$$

- Evaluate the derivative and set to zero, we have

$$q'(x) = f'(x_n) + f''(x_n)(x - x_n) = 0$$

- Solve for the next iterate:

$$x_{n+1} = x_n - \frac{f'(x_n)}{f''(x_n)}$$

- The multivariate second order Taylor expansion of $f(\mathbf{x})$ w.r.t. $\mathbf{x}^{(k)}$ is

$$f(\mathbf{x}) \approx q(\mathbf{x}) = f(\mathbf{x}^{(k)}) + {\mathbf{g}^{(k)}}^\top (\mathbf{x} - \mathbf{x}^{(k)}) + \frac{1}{2}(\mathbf{x} - \mathbf{x}^{(k)})^\top \mathbf{H}^{(k)} (\mathbf{x} - \mathbf{x}^{(k)})$$

  where $\mathbf{g}^{(k)}$, $\mathbf{H}^{(k)}$ are the local gradient and Hessian resp.

- Evaluate the gradient and set to zero, we have

$$\nabla q(\mathbf{x}) = \mathbf{g}^{(k)} + \mathbf{H}^{(k)}(\mathbf{x} - \mathbf{x}^{(k)}) = 0$$

- Solve for the next iterate:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} - {\mathbf{H}^{(k)}}^{-1} \mathbf{g}^{(k)}$$

Numerical Differentiation: Finite Difference

$$f'(x) \approx \underbrace{\frac{f(x+h)-f(x)}{h}}_{\text{forward difference}} \approx \underbrace{\frac{f(x+\frac{h}{2})-f(x-\frac{h}{2})}{h}}_{\text{central difference}} \approx \underbrace{\frac{f(x)-f(x-h)}{h}}_{\text{backward difference}}$$

Numerical Differentiation: Complex Step Method

- $f(x+ih) = f(x) + ihf'(x) - h^2\frac{f''(x)}{2!} - ih^3\frac{f'''(x)}{3!} + \cdots$
- Take the imaginary part: $\operatorname{Im} f(x+ih) = hf'(x) - h^3\frac{f'''(x)}{3!} + \cdots \implies f'(x) \approx \frac{\operatorname{Im} f(x+ih)}{h} + \mathcal{O}(h^2)$
- Take the real part: $\operatorname{Re} f(x+ih) = f(x) - h^2\frac{f''(x)}{2!} + \cdots \implies f(x) \approx \operatorname{Re} f(x+ih) + \mathcal{O}(h^2)$

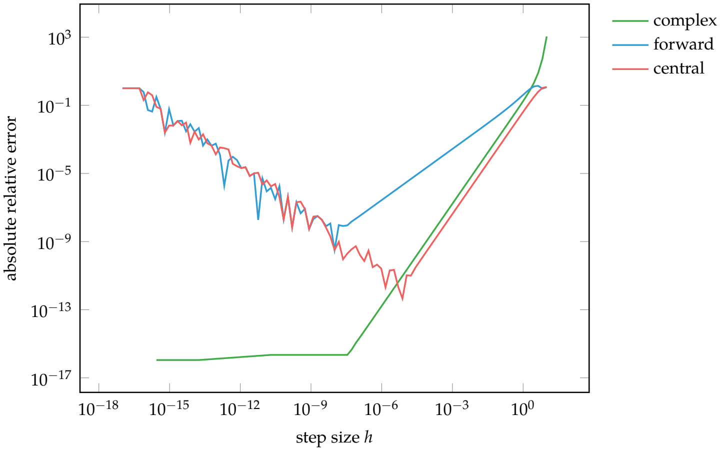

Figure 1: Evaluation of the numerical derivative of $\sin x$ at $x = \frac{1}{2}$ via different schemes as the step size h is varied.

Automatic Differentiation (AD)

- No round-off errors in numerical differentiation
- NOT symbolic differentiation of computer algebra systems
- Every computer calculation executes a sequence of elementary arithmetic operations ($+$, $-$, $\times$, $\div$, composite) and elementary functions (e.g. exp, log, sin, cos, etc.).
- Applying the chain rule repeatedly; partial derivatives of arbitrary order can be computed automatically
- Accurately to working precision, and using at most a small constant factor of more arithmetic operations than the original program
- Indispensable for modern applications, many implementations: e.g. `autograd`, `JAX`
- Two modes: forward and reverse
- Blog post about fine points of AD and implementations
- References: Naumann (2012); Griewank and Walther (2008)

AD: Forward Mode

Example. Given $z = x_1 x_2 + \sin x_1$, compute $\dfrac{\partial z}{\partial x_1}$ at $x_1 = 1.5$, $x_2 = 0.5$.

Solution.

Intermediate Var.	Expression	Value	Derivative
w_1	x_1	1.5	1
w_2	x_2	0.5	0
w_3	$w_1 w_2$	0.75	0.5
w_4	$\sin w_1$	0.9974	0.07
w_5	$w_3 + w_4$	1.7474	0.57

$$\frac{\partial w_3}{\partial x_1} = \frac{\partial w_3}{\partial w_1}\frac{\partial w_1}{\partial x_1} + \frac{\partial w_3}{\partial w_2}\frac{\partial w_2}{\partial x_1} = w_2 \cdot 1 + w_1 \cdot 0 = 0.5$$
$$\frac{\partial w_4}{\partial x_1} = \frac{\partial w_4}{\partial w_1}\frac{\partial w_1}{\partial x_1} = \cos w_1 \cdot 1 = \cos(1.5) = 0.07$$

Example (Griewank and Walther (2008) pp.5). $y = \left(\sin\frac{x_1}{x_2} + \frac{x_1}{x_2} - e^{x_2}\right) \cdot \left(\frac{x_1}{x_2} - e^{x_2}\right)$, compute $\frac{\partial y}{\partial x_1}$ at $x_1 = 1.5$, $x_2 = 0.5$.

Solution.

Intermediate Var.	Expression	Value	Derivative
w_1	x_1	1.5	1
w_2	x_2	0.5	0
w_3	$\frac{w_1}{w_2}$	3	2
w_4	$\sin w_3$	0.1411	−1.98
w_5	e^{w_2}	1.6487	0
w_6	$w_3 - w_5$	1.3513	2
w_7	$w_4 + w_6$	1.4924	0.02
w_8	$w_6 w_7$	2.0167	3.0118

$$\frac{\partial w_3}{\partial x_1} = \frac{\partial w_3}{\partial w_1}\frac{\partial w_1}{\partial x_1} + \frac{\partial w_3}{\partial w_2}\frac{\partial w_2}{\partial x_1} = \frac{1}{w_2} \cdot 1 + \frac{-w_1}{w_2^2} \cdot 0 = \frac{1}{w_2} = \frac{1}{0.5} = 2$$

$$\frac{\partial w_4}{\partial x_1} = \frac{\partial w_4}{\partial w_3}\frac{\partial w_3}{\partial x_1} = \cos w_3 \cdot \frac{1}{w_2} = \frac{\cos 3}{0.5} = \frac{-0.99}{0.5} = -1.98$$

AD: Reverse Mode

Example. Given $z = x_1 x_2 + \sin x_1$, compute $\dfrac{\partial z}{\partial x_1}$ at $x_1 = 1.5$, $x_2 = 0.5$.

Solution. Set

$$\begin{aligned} w_1 &= x_1 \\ w_2 &= x_2 \\ w_3 &= w_1 w_2 \\ w_4 &= \sin w_1 \\ w_5 &= w_3 + w_4 \\ z &= w_5 \end{aligned}$$

$$\begin{aligned} \frac{\partial z}{\partial x_1} = \frac{\partial z}{\partial w_1} = \frac{\partial w_5}{\partial w_1} &= \frac{\partial w_5}{\partial w_3}\frac{\partial w_3}{\partial w_1} + \frac{\partial w_5}{\partial w_4}\frac{\partial w_4}{\partial w_1} \\ &= w_2 + \cos w_1 = 0.5 + \cos(1.5) = 0.5 + 0.07 = 0.57 \end{aligned}$$

Example (Griewank and Walther (2008) pp.5). $y = \left(\sin\frac{x_1}{x_2} + \frac{x_1}{x_2} - e^{x_2}\right) \cdot \left(\frac{x_1}{x_2} - e^{x_2}\right)$, compute $\frac{\partial y}{\partial x_1}$ at $x_1 = 1.5$, $x_2 = 0.5$.

Solution. Set

$$w_1 = x_1, \quad w_2 = x_2, \quad w_3 = \frac{w_1}{w_2}, \quad w_4 = \sin w_3, \quad w_5 = e^{w_2}$$

$$w_6 = w_3 - w_5, \quad w_7 = w_4 + w_6, \quad w_8 = w_6 \cdot w_7, \quad y = w_8$$

$\frac{\partial y}{\partial x_1} = \frac{\partial y}{\partial w_1} = \frac{\partial w_8}{\partial w_1} = \frac{\partial w_8}{\partial w_6}\frac{\partial w_6}{\partial w_1} + \frac{\partial w_8}{\partial w_7}\frac{\partial w_7}{\partial w_1} = w_7\frac{\partial w_6}{\partial w_1} + w_6\frac{\partial w_7}{\partial w_1}$
$= w_7\frac{\partial w_6}{\partial w_1} + w_6\left(\frac{\partial w_4}{\partial w_1} + \frac{\partial w_6}{\partial w_1}\right) = (w_7 + w_6)\left(\frac{\partial w_3}{\partial w_1} - \frac{\partial w_5}{\partial w_1}\right) + w_6\left(\frac{\partial w_4}{\partial w_1}\right)$
$= (w_7 + w_6)\frac{\partial w_3}{\partial w_1} + w_6\frac{\partial w_4}{\partial w_3}\frac{\partial w_3}{\partial w_1} = (w_7 + w_6(1 + \cos w_3))\frac{\partial w_3}{\partial w_1}$
$= \frac{w_7 + w_6(1 + \cos w_3)}{w_2}$. Now $w_1 = x_1 = 1.5$, $w_2 = x_2 = 0.5$, $w_3 = 3$, $w_4 = 0.1411$, $w_5 = 1.6487$, $w_6 = 3 - 1.6487 = 1.3513$, $w_7 = 0.1411 + 1.3513 = 1.4924$, so $\frac{\partial y}{\partial x_1} = \frac{1.4924 + 1.3513 \cdot (1 + \cos 3)}{0.5} = 3.0118$. ($\cos 3 = -0.99$)

Choosing Forward / Reverse Mode

- The chain rule: the Jacobian of a operation is the matrix multiplication of all the Jacobians of sub-operations
- Let $\mathbf{y} = f(\mathbf{x}) = r(q(p(\mathbf{x})))$ and $\mathbf{a} = p(\mathbf{x})$, $\mathbf{b} = q(\mathbf{a})$, $y = r(\mathbf{b})$; the Jacobian reads

$$\underbrace{\frac{\partial \mathbf{y}}{\partial \mathbf{x}}}_{|\mathbf{y}|\times|\mathbf{x}|} = \underbrace{\frac{\partial r(\mathbf{b})}{\partial \mathbf{b}}}_{|\mathbf{y}|\times|\mathbf{b}|} \underbrace{\frac{\partial q(\mathbf{a})}{\partial \mathbf{a}}}_{|\mathbf{b}|\times|\mathbf{a}|} \underbrace{\frac{\partial p(\mathbf{x})}{\partial \mathbf{x}}}_{|\mathbf{a}|\times|\mathbf{x}|}$$

- The number of scalar multiplications required to multiply two matrices of sizes $\alpha \times \beta$ and $\beta \times \gamma$ is $\alpha \cdot \beta \cdot \gamma$
- Forward mode: $\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \frac{\partial r(\mathbf{b})}{\partial \mathbf{b}} \left(\frac{\partial q(\mathbf{a})}{\partial \mathbf{a}} \frac{\partial p(\mathbf{x})}{\partial \mathbf{x}} \right)$, $|\mathbf{b}| \cdot |\mathbf{a}| \cdot |\mathbf{x}| + |\mathbf{y}| \cdot |\mathbf{b}| \cdot |\mathbf{x}|$ multiplications
- Reverse mode: $\frac{\partial \mathbf{y}}{\partial \mathbf{x}} = \left(\frac{\partial r(\mathbf{b})}{\partial \mathbf{b}} \frac{\partial q(\mathbf{a})}{\partial \mathbf{a}} \right) \frac{\partial p(\mathbf{x})}{\partial \mathbf{x}}$, $|\mathbf{y}| \cdot |\mathbf{b}| \cdot |\mathbf{a}| + |\mathbf{y}| \cdot |\mathbf{a}| \cdot |\mathbf{x}|$ multiplications
- Assume $|\mathbf{a}| = |\mathbf{b}|$. If $|\mathbf{y}| > |\mathbf{x}|$, forward mode involves fewer steps; else if $|\mathbf{y}| < |\mathbf{x}|$, reverse mode involves fewer steps

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