APM462
Lecture Notes

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December 15, 2019

Contents

1 Matrix Calculus

Row v.s. Column Vector Our default rule is that every vector is a column vector unless explicitly stated otherwise.
This is also known as the numerator layout.
Special case: For $f : \mathbb{R}^n \to \mathbb{R}$, Df is a $1 \times n$ matrix or row vector.

1.1 Matrix Multiplication

Definition 1.1.1 Let A be $m \times n$, and B be $n \times p$, and let the product AB be

$$C = AB$$

then C is a $m \times p$ matrix, with element (i, j) given by

$$c_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj}$$

for all $i = 1, 2, \ldots, m, j = 1, 2, \ldots, p$.

Proposition 1.1.2 Let A be $m \times n$, and x be $n \times 1$, then the typical element of the product

$$z = Ax$$

is given by

$$z_i = \sum_{k=1}^{n} a_{ik} x_k$$

for all $i = 1, 2, \ldots, m$.
Similarly, let y be $m \times 1$, then the typical element of the product

$$z^T = y^T A$$

is given by

$$z_i^T = \sum_{k=1}^{n} a_{ki} y_k$$

for all $i = 1, 2, \ldots, n$.
Finally, the scalar resulting from the product

$$\alpha = y^T A x$$

is given by

$$\alpha = \sum_{j=1}^{m} \sum_{k=1}^{n} a_{jk} y_i x_k$$

1.2 Partitioned Matrices

Proposition 1.2.1 Let A be a square, nonsingular matrix of order m. Partition A as

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$$

so that A_{11} and A_{22} are invertible.
Then

$$A^{-1} = \begin{bmatrix} (A_{11} - A_{12}A_{22}^{-1}A_{21})^{-1} & -A_{11}^{-1}A_{12}(A_{22} - A_{21}A_{11}^{-1}A_{12})^{-1} \\ -A_{22}^{-1}A_{21}(A_{11} - A_{12}A_{22}^{-1}A_{21})^{-1} & (A_{22} - A_{21}A_{11}^{-1}A_{12})^{-1} \end{bmatrix}$$

proof:
Direct multiplication of the proposed A^{-1} and A yields

$$A^{-1}A = I$$

■

1.3 Matrix Differentiation

Proposition 1.3.1

$$\frac{\partial A}{\partial x} = \frac{\partial A^T}{\partial x}$$

Proposition 1.3.2 Let

$$y = Ax$$

where y is $m \times 1$, x is $n \times 1$, A is $m \times n$, and A does not depend on x. Suppose that x is a function of the vector z, while A is independent of z. Then

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

Proposition 1.3.3 Let the scalar α be defined by

$$\alpha = y^T Ax$$

where y is $m \times 1$, x is $n \times 1$, A is $m \times n$, and A is independent of x and y, then

$$\frac{\partial \alpha}{\partial x} = y^T A$$

and

$$\frac{\partial \alpha}{\partial y} = x^T A^T$$

Proposition 1.3.4 For the special case where the scalar α is given by the quadratic form

$$\alpha = x^T Ax$$

where x is $n \times 1$, A is $n \times n$, and A does not depend on x, then

$$\frac{\partial \alpha}{\partial x} = x^T(A + A^T)$$

proof:
By definition

$$\alpha = \sum_{j=1}^{n}\sum_{i=1}^{n} a_{ij}x_i x_j$$

Differentiating with respect to the kth element of x we have

$$\frac{\partial \alpha}{\partial x_k} = \sum_{j=1}^{n} a_{kj}x_J + \sum_{i=1}^{n} a_{ik}x_i$$

for all $k = 1, 2, \ldots, n$, and consequently,

$$\frac{\partial \alpha}{\partial x} = x^T A^T + x^T A = x^T(A^T + A)$$

■

Proposition 1.3.4 For the special case where A is a symmetric matrix and

$$\alpha = x^T Ax$$

where x is $n \times 1$, A is $n \times n$, and A does not depend on x, then

$$\frac{\partial \alpha}{\partial x} = 2x^T A$$

Proposition 1.3.5 Let the scalar α be defined by

$$\alpha = y^T x$$

where y is $n \times 1$, x is $n \times 1$, and both y and x are functions of the vector z. Then

$$\frac{\partial \alpha}{\partial z} = x^T \frac{\partial y}{\partial z} + y^T \frac{\partial x}{\partial z}$$

Proposition 1.3.6 Let the scalar α be defined by

$$\alpha = x^T x$$

where x is $n \times 1$, and x is a functions of the vector z. Then

$$\frac{\partial \alpha}{\partial z} = 2x^T \frac{\partial y}{\partial z}$$

Proposition 1.3.7 Let the scalar α be defined by

$$\alpha = y^T A x$$

where y is $m \times 1$, A is $m \times n$, x is $n \times 1$, and both y and x are functions of the vector z, while A does not depend on z. Then

$$\frac{\partial \alpha}{\partial z} = x^T A^T \frac{\partial y}{\partial z} + y^T A \frac{\partial x}{\partial z}$$

Proposition 1.3.8 Let A be an invertible, $m \times m$ matrix whose elements are functions of the scalar parameter α. Then

$$\frac{\partial A^{-1}}{\partial \alpha} = -A^{-1} \frac{\partial A}{\partial \alpha} A^{-1}$$

proof:
Start with the definition of the inverse

$$A^{-1} A = I$$

and differentiate, yielding

$$A^{-1} \frac{\partial A}{\partial \alpha} + \frac{\partial A^{-1}}{\partial \alpha} A = 0$$

rearranging the terms yields

$$\frac{\partial A^{-1}}{\partial \alpha} = -A^{-1} \frac{\partial A}{\partial \alpha} A^{-1}$$

■

Vector-by-vector Differentiation Identities 1.3.9

Young's Theorem 1.3.10 i.e. Symmetry of second derivatives

$$[\nabla_{xy} f(x, y)]^T = \nabla_{yx} f(x, y)$$

proof:
This is straightforward by writing out the elements of the matrix. ■

2 Second-year Calculus Review

functions $\mathbb{R} \to \mathbb{R}$

Condition	Expression	Numerator layout, i.e. by y and $\mathbf{x}^\mathsf{T}$	Denominator layout, i.e. by $\mathbf{y}^\mathsf{T}$ and x
a is not a function of **x**	$\frac{\partial \mathbf{a}}{\partial \mathbf{x}} =$	$\mathbf{0}$	
	$\frac{\partial \mathbf{x}}{\partial \mathbf{x}} =$	$\mathbf{I}$	
A is not a function of **x**	$\frac{\partial \mathbf{A}\mathbf{x}}{\partial \mathbf{x}} =$	$\mathbf{A}$	$\mathbf{A}^\top$
A is not a function of **x**	$\frac{\partial \mathbf{x}^\top \mathbf{A}}{\partial \mathbf{x}} =$	$\mathbf{A}^\top$	$\mathbf{A}$
a is not a function of **x**, **u** = **u**(**x**)	$\frac{\partial a\mathbf{u}}{\partial \mathbf{x}} =$	$a\frac{\partial \mathbf{u}}{\partial \mathbf{x}}$	
v = *v*(**x**), **u** = **u**(**x**)	$\frac{\partial v\mathbf{u}}{\partial \mathbf{x}} =$	$v\frac{\partial \mathbf{u}}{\partial \mathbf{x}} + \mathbf{u}\frac{\partial v}{\partial \mathbf{x}}$	$v\frac{\partial \mathbf{u}}{\partial \mathbf{x}} + \frac{\partial v}{\partial \mathbf{x}}\mathbf{u}^\top$
A is not a function of **x**, **u** = **u**(**x**)	$\frac{\partial \mathbf{A}\mathbf{u}}{\partial \mathbf{x}} =$	$\mathbf{A}\frac{\partial \mathbf{u}}{\partial \mathbf{x}}$	$\frac{\partial \mathbf{u}}{\partial \mathbf{x}}\mathbf{A}^\top$
u = **u**(**x**), **v** = **v**(**x**)	$\frac{\partial (\mathbf{u}+\mathbf{v})}{\partial \mathbf{x}} =$	$\frac{\partial \mathbf{u}}{\partial \mathbf{x}} + \frac{\partial \mathbf{v}}{\partial \mathbf{x}}$	
u = **u**(**x**)	$\frac{\partial \mathbf{g}(\mathbf{u})}{\partial \mathbf{x}} =$	$\frac{\partial \mathbf{g}(\mathbf{u})}{\partial \mathbf{u}}\frac{\partial \mathbf{u}}{\partial \mathbf{x}}$	$\frac{\partial \mathbf{u}}{\partial \mathbf{x}}\frac{\partial \mathbf{g}(\mathbf{u})}{\partial \mathbf{u}}$
u = **u**(**x**)	$\frac{\partial \mathbf{f}(\mathbf{g}(\mathbf{u}))}{\partial \mathbf{x}} =$	$\frac{\partial \mathbf{f}(\mathbf{g})}{\partial \mathbf{g}}\frac{\partial \mathbf{g}(\mathbf{u})}{\partial \mathbf{u}}\frac{\partial \mathbf{u}}{\partial \mathbf{x}}$	$\frac{\partial \mathbf{u}}{\partial \mathbf{x}}\frac{\partial \mathbf{g}(\mathbf{u})}{\partial \mathbf{u}}\frac{\partial \mathbf{f}(\mathbf{g})}{\partial \mathbf{g}}$

2.1 Mean Value Theorem in 1 Dimension

$g \in C^1$ on $\mathbb{R}$

$$\frac{g(x+h)-g(x)}{h} = g'(x+\theta h)$$

where $\theta \in (0,1)$
Or equivalently,

$$g(x+h) = g(x) + hg'(x+\theta h)$$

2.2 1st Order Taylor Approximation

$g \in C^1$ on $\mathbb{R}$

$$g(x+h) = g(x) + hg'(x) + o(h)$$

where $o(h)$ is "little o" of h, the error term.
Say a function $f(h) = o(h)$, this means $\lim_{h\to 0}\frac{f(h)}{h} = 0$
For example, for $f(h) = h^2$, we can say $f(h) = o(h)$,
since $\lim_{h\to 0}\frac{f(h)}{h} = \lim_{h\to 0}\frac{h^2}{h} = \lim_{h\to 0} h = 0$
proof: (Use MVT):
WTS : $g(x+h) - g(x) - hg'(x) = o(h)$

$$\begin{aligned}\lim_{h\to 0}\frac{[g(x+h)-g(x)]-hg'(x)}{h} &= \lim_{h\to 0}\frac{[hg'(x+\theta h)]-hg'(x)}{h}\\ &= \lim_{h\to 0} g'(x+\theta h) - g'(x)\\ &= \lim_{h\to 0} g'(x) - g'(x)\\ &= 0\end{aligned}$$

■

2.3 2nd Order Mean Value Theorem

$g \in C^2$ on $\mathbb{R}$

$$g(x+h) = g(x) + hg'(x) + \frac{h^2}{2}g'(x+\theta h)$$

for some $\theta \in (0,1)$

proof:
WTS: $g(x+h) - g(x) - hg'(x) - \frac{h^2}{2}g''(x) = o(h^2)$

$$\begin{aligned}
\lim_{h\to 0} \frac{g(x+h) - g(x) - hg'(x) - \frac{h^2}{2}g''(x)}{h^2} &= \lim_{h\to 0} \frac{[\frac{h^2}{2}g'(x+\theta h)] - \frac{h^2}{2}g''(x)}{h^2} \\
&= \lim_{h\to 0} \frac{1}{2}(g''(x+\theta h) - g''(x)) \\
&= \lim_{h\to 0} \frac{1}{2}(g''(x) - g''(x)) \\
&= 0
\end{aligned}$$

■

multivariate functions: $\mathbb{R}^n \to \mathbb{R}$

2.4 Recall: Definition of gradient

Gradient of $f : \mathbb{R}^n \to \mathbb{R}$ at $x \in \mathbb{R}^n$ (denoted $\nabla f(x)$) if exists is a vector characterized by the property:

$$\lim_{\mathbf{v}\to\mathbf{0}} \frac{f(\mathbf{x}+\mathbf{v}) - f(\mathbf{x}) - \nabla f(\mathbf{x}) \cdot \mathbf{v}}{||\mathbf{v}||} = 0$$

In Cartesian coordinates, $\nabla f(\mathbf{x}) = (\frac{\partial f}{\partial \mathbf{x}_1}(\mathbf{x}), \ldots, \frac{\partial f}{\partial \mathbf{x}_n}(\mathbf{x}))$

2.5 Mean Value Theorem in n dimension

$f \in C^1$ on $\mathbb{R}^n$, then for any $\mathbf{x}, \mathbf{v} \in \mathbb{R}^n$,

$$f(\mathbf{x}+\mathbf{v}) = f(\mathbf{x}) + \nabla f(\mathbf{x}+\theta\mathbf{v}) \cdot \mathbf{v}$$

for some $\theta \in (0,1)$

proof: Reduce to 1-dimension case
$g(t) := f(\mathbf{x}+t\mathbf{v}), t \in \mathbb{R}$

$$\begin{aligned}
g'(t) &= \frac{d}{dt} f(\mathbf{x}+t\mathbf{v}) \\
&= \sum_{i=1}^{n} \frac{\partial f}{\partial \mathbf{x}_i}(\mathbf{x}+t\mathbf{v}) \cdot \frac{d(\mathbf{x}+t\mathbf{v})_i}{dt} && \text{(by Chain Rule)} \\
&= \sum \frac{\partial f}{\partial \mathbf{x}_i}(\mathbf{x}+t\mathbf{v}) \cdot \frac{d(\mathbf{x}_i + t\mathbf{v}_i)}{dt} \\
&= \sum \frac{\partial f}{\partial \mathbf{x}_i}(\mathbf{x}+t\mathbf{v}) \cdot \mathbf{v}_i \\
&= \nabla f(\mathbf{x}+t\mathbf{v}) \cdot \mathbf{v} && (*)
\end{aligned}$$

$g \in C^1$ on $\mathbb{R}$
Using MVT in $\mathbb{R}$:

$$\begin{aligned} f(\mathbf{x}+\mathbf{v}) &= g(1) \\ &= g(0+1) \\ &= g(0) + 1g'(0+\theta 1) && (\theta \in (0,1)) \\ &= g(0) + g'(\theta) \\ &= f(\mathbf{x}) + \nabla f(\mathbf{x}+\theta\mathbf{v}) \cdot \mathbf{v} && (\text{by } (*)) \end{aligned}$$

■

2.6 1st Order Taylor Approximation in $\mathbb{R}^n$

$f \in C^1$ on $\mathbb{R}^n$

$$f(\mathbf{x}+\mathbf{v}) = f(\mathbf{x}) + \nabla f(\mathbf{x}) \cdot \mathbf{v} + o(||\mathbf{v}||)$$

proof:

$$\begin{aligned} \lim_{||\mathbf{v}||\to 0} \frac{[f(\mathbf{x}+\mathbf{v}) - f(\mathbf{x})] - \nabla f(\mathbf{x}) \cdot \mathbf{v}}{||\mathbf{v}||} &= \lim_{||\mathbf{v}||\to 0} \frac{[\nabla f(\mathbf{x}+\theta\mathbf{v}) \cdot \mathbf{v}] - \nabla f(\mathbf{x}) \cdot \mathbf{v}}{||\mathbf{v}||} \\ &= \lim_{||\mathbf{v}||\to 0} [\nabla f(\mathbf{x}+\theta\mathbf{v}) - \nabla f(\mathbf{x})] \cdot \frac{\mathbf{v}}{||\mathbf{v}||} \\ &= 0 && (\tfrac{\mathbf{v}}{||\mathbf{v}||} \text{ is a unit vector, remains 1}) \end{aligned}$$

■

2.7 2nd Order Mean Value Theorem in $\mathbb{R}^n$

$f \in C^2$ on $\mathbb{R}^n$

$$f(\mathbf{x}+\mathbf{v}) = f(\mathbf{x}) + \nabla f(\mathbf{x}) \cdot \mathbf{v} + \frac{1}{2}\mathbf{v}^T \nabla^2 f(\mathbf{x}+\theta\mathbf{v}) \cdot \mathbf{v}$$

Remarks In this course, ∇^2 means Hessian, not Laplacian.

$$\nabla^2 f(\mathbf{x}) = \left(\frac{\partial^2 f}{\partial \mathbf{x}_i \partial \mathbf{x}_j}\right)_{1\le i,j\le n}(\mathbf{x}) = \begin{pmatrix} \frac{\partial f}{\partial_1^2} & \frac{\partial f}{\partial_1 \partial_2} & \cdots \\ \frac{\partial f}{\partial_2 \partial_1} & \cdots & \\ \vdots & & \end{pmatrix}$$

The Hessian matrix is symmetric. This is sometimes called Clairaut's Theorem.
note: $\mathbf{v}^T \nabla^2 f(\mathbf{x}) \mathbf{v} = \sum_{1\le i,j\le n} \frac{\partial^2 f}{\partial \mathbf{x}_i \partial \mathbf{x}_j} f(\mathbf{x}) \mathbf{v}_i \mathbf{v}_j$

2.8 2nd Order Taylor Approximation in $\mathbb{R}^n$

$f \in C^2$ on $\mathbb{R}^n$

$$f(\mathbf{x}+\mathbf{v}) = f(\mathbf{x}) + \nabla f(\mathbf{x}) \cdot \mathbf{v} + \frac{1}{2}\mathbf{v}^T \nabla^2 f(\mathbf{x}) \mathbf{v} + o(||\mathbf{v}||^2)$$

proof:

$$\lim_{||\mathbf{v}||\to 0}\frac{[f(\mathbf{x}+\mathbf{v})-f(\mathbf{x})]-\nabla f(\mathbf{x})\cdot\mathbf{v}-\frac{1}{2}\mathbf{v}^T\nabla^2 f(\mathbf{x})\mathbf{v}}{||\mathbf{v}||^2}=\lim_{||\mathbf{v}||\to 0}\frac{[\frac{1}{2}\mathbf{v}^T\nabla^2 f(\mathbf{x}+\theta\mathbf{v})\cdot\mathbf{v}]-\frac{1}{2}\mathbf{v}^T\nabla^2 f(\mathbf{x})\cdot\mathbf{v}}{||\mathbf{v}||^2}$$

(By 2nd MVT)

$$=\lim_{||\mathbf{v}||\to 0}\frac{1}{2}(\frac{\mathbf{v}}{||\mathbf{v}||})^T[\nabla^2 f(\mathbf{x}+\theta\mathbf{v})-\nabla^2 f(\mathbf{x})](\frac{\mathbf{v}}{||\mathbf{v}||})$$

$$=0$$

■

2.9 Geometric Meaning of Gradient

$f:\mathbb{R}^n\to\mathbb{R}$
Rate of change of f at $\mathbf{x}$ in direction $\mathbf{v}\,(||\mathbf{v}||=1)=\frac{d}{dt}|_{t=0}f(\mathbf{x}+t\mathbf{v})$

$$\begin{aligned}\frac{d}{dt}|_{t=0}f(\mathbf{x}+t\mathbf{v})&=\nabla f(\mathbf{x}+t\mathbf{v})\cdot\mathbf{v}|_{t=0}\\&=\nabla f(\mathbf{x})\cdot\mathbf{v}\\&=|\nabla f(\mathbf{x})||\mathbf{v}|\cos\theta\\&=|\nabla f(\mathbf{x})|\cos\theta\qquad(||\mathbf{v}||=1)\end{aligned}$$

maximized at $\theta=0$
So $\nabla f(\mathbf{x})$ points in the direction of steepest ascent.

2.10 Implicit Function Theorem

$f:\mathbb{R}^{n+1}\to\mathbb{R}\in C^1$
Fix $(\mathbf{a},b)\in\mathbb{R}^n\times\mathbb{R}$ s.t. $f(\mathbf{a},b)=0$.
If $\nabla f(\mathbf{a},b)\neq 0$, then $\{(\mathbf{x},y)\in(\mathbb{R}^n\times\mathbb{R})|f(\mathbf{x},y)=0\}$ is locally (near $(\mathbf{a},b)$) the graph of a function.

2.11 Level Sets of f

c-level set of $f:=\{\mathbf{x}\in\mathbb{R}^n|f(\mathbf{x})=c\}$

Fact gradient $\nabla f(\mathbf{x}_0)\perp$ level curve (through $\mathbf{x}_0$)

3 Convex Sets & Functions

3.1 Definitions

Definition of Convex Set $\Omega\subseteq\mathbb{R}^n$ is a convex set if $\mathbf{x}_1,\mathbf{x}_2\in\Omega\Rightarrow s\mathbf{x}_1+(1-s)\mathbf{x}_2\in\Omega$ where $s\in[0,1]$

Definition of Convex Function A function $f:$ convex $\Omega\subseteq\mathbb{R}^n$ is convex if

$$f(s\mathbf{x}_1+(1-s)\mathbf{x}_2)\leq sf(\mathbf{x}_1)+(1-s)f(\mathbf{x}_2)$$

for all $\mathbf{x}_1,\mathbf{x}_2\in\Omega$ and all $s\in[0,1]$

Remarks Second line above (or equal to) the graph

Definition of Concave Function A function f is concave if $-f$ is convex.

3.2 Basic Properties of Convex Functions

Let $\Omega \subseteq \mathbb{R}^n$ be a convex set.

1. f_1, f_2 are convex functions on $\Omega \Rightarrow f_1 + f_2$ is a convex function on Ω.
2. f is a convex function, $a \geq 0 \Rightarrow af$ is a convex function.
3. f is a convex function on $\Omega \Rightarrow$ The sublevel sets of f, $SL_c := \{\mathbf{x} \in \mathbb{R}^n | f(\mathbf{x}) \leq c\}$ is convex.

proof of (3):
Let $x_1, x_2 \in SL_C$, so that $f(x_1) \leq c$ and $f(x_2) \leq c$.
WTS: $sx_1 + (1-s)x_2 \in SL_c$ for any $s \in [0,1]$

$$\begin{aligned} f(sx_1 + (1-s)x_2) &\leq sf(x_1) + (1-s)f(x_2) && (f \text{ is convex}) \\ &\leq sc + (1-s)c \\ &= c \\ \Rightarrow sx_1 + (1-s)x_2 &\in SL_c \end{aligned}$$

■

Example of a convex function Let $f : \mathbb{R} \to \mathbb{R}$, $f(x) = |x|$
Let $x_1, x_2 \in \mathbb{R}, s \in [0,1]$
Then

$$\begin{aligned} f(sx_1 + (1-s)x_2) &= |sx_1 + (1-s)x_2| \\ &\leq |sx_1| + |(1-s)x_2| && \text{(by Triangle Inequality)} \\ &= s|x_1| + (1-s)|x_2| \\ &= sf(x_1) + (1-s)f(x_2) \end{aligned}$$

Then f is a convex function.

Theorem - Characterization of C^1 convex functions Let f : convex subset of $\mathbb{R}^n$ $\Omega \to \mathbb{R}$ be a C^1 function.
Then,
f is convex $\iff$ $f(y) \geq f(x) + \nabla f(x) \cdot (y - x)$ for all $x, y \in \Omega$

Remarks Tangent line below the graph.

proof:
($\Rightarrow$)
f is convex, then by definition,

$$\begin{aligned} f(s\mathbf{x}_1 + (1-s)\mathbf{x}_2) &\leq sf(\mathbf{x}_1) + (1-s)f(\mathbf{x}_2) \\ f(s\mathbf{x}_1 + (1-s)\mathbf{x}_2) - f(\mathbf{x}_2) &\leq s(f(\mathbf{x}_1) - f(\mathbf{x}_2)) \\ \frac{f(s\mathbf{x}_1 + (1-s)\mathbf{x}_2) - f(\mathbf{x}_2)}{s} &\leq f(\mathbf{x}_1) - f(\mathbf{x}_2) \\ \lim_{s \to 0} \frac{f(\mathbf{x}_2 + s(\mathbf{x}_1 - \mathbf{x}_2)) - f(\mathbf{x}_2)}{s} &\leq f(\mathbf{x}_1) - f(\mathbf{x}_2) \\ \nabla f(\mathbf{x}_2) \cdot (\mathbf{x}_1 - \mathbf{x}_2) &\leq f(\mathbf{x}_1) - f(\mathbf{x}_2) \qquad (\text{since } \tfrac{d}{ds}|_{s=0} f(\mathbf{x}_2 + s(\mathbf{x}_1 - \mathbf{x}_2)) = \nabla f(\mathbf{x}_2) \cdot (\mathbf{x}_1 - \mathbf{x}_2)) \\ f(\mathbf{x}_2) + \nabla f(\mathbf{x}_2) \cdot (\mathbf{x}_1 - \mathbf{x}_2) &\leq f(\mathbf{x}_1) \\ f(\mathbf{x}) + \nabla f(\mathbf{x}) \cdot (\mathbf{y} - \mathbf{x}) &\leq f(\mathbf{y}) \end{aligned}$$

where $0 \leq s \leq 1$
($\Leftarrow$)
Fix $\mathbf{x}_0, \mathbf{x}_1 \in \Omega$ and $s \in (0,1)$
Let $x = s\mathbf{x}_0 + (1-s)\mathbf{x}_1$

$$\begin{cases} f(\mathbf{x}_0) & \geq f(\mathbf{x}) + \nabla f(\mathbf{x}) \cdot (\mathbf{x}_0 - \mathbf{x}) \\ & = f(\mathbf{x}) + \nabla f(\mathbf{x}) \cdot (1-s)(\mathbf{x}_0 - \mathbf{x}_1) \\ f(\mathbf{x}_1) & \geq f(\mathbf{x}) + \nabla f(\mathbf{x}) \cdot (\mathbf{x}_1 - \mathbf{x}) \\ & = f(\mathbf{x}) + \nabla f(\mathbf{x}) \cdot s(\mathbf{x}_1 - \mathbf{x}_0) \end{cases}$$

$$\begin{cases} sf(x_0) & \geq sf(\mathbf{x}) + \nabla f(\mathbf{x}) \cdot (1-s) \cdot s(\mathbf{x}_0 - \mathbf{x}_1) \\ (1-s)f(\mathbf{x}_1) & \geq (1-s)f(\mathbf{x}) + \nabla f(\mathbf{x}) \cdot (1-s) \cdot s(\mathbf{x}_1 - \mathbf{x}_0) \end{cases}$$

Then

$$sf(\mathbf{x}_0) + (1-s)f(\mathbf{x}_1) \geq f(x) + 0$$

Then f is convex. ■

3.3 Criterions for convexity

C^1 criterion for convexity

$$f : \Omega \to \mathbb{R} \text{ is convex} \iff f(y) \geq f(x) + \nabla f(x) \cdot (y - x)$$

for all $x, y \in \Omega$

Theorem: C^2 criterion for convexity Let $f \in C^2$ on $\Omega \subseteq \mathbb{R}^n$ (here we assume $\Omega \subseteq \mathbb{R}^n$ is a convex set containing an interior point)
Then

$$f \text{ is convex on } \Omega \iff \nabla^2 f(x) \geq 0$$

for all $x \in \Omega$

Remark 1 Let A be an $n \times n$ matrix.
"$A \geq 0$" means A is positive semi-definite:

$$v^T A v \geq 0$$

for all $v \in \mathbb{R}^n$

Remark 2 In $\mathbb{R}$,

$$f \text{ is convex} \iff f'(x) \geq 0$$

for all $x \in \Omega$
("concave up" in first year calculus)

proof for Theorem:
Recall 2nd order MVT:

$$f(y) = f(x) + \nabla f(x) \cdot (y - x) + \frac{1}{2}(y - x)^T \nabla^2 f(x + s(y - x)) \cdot (y - x)$$

for some $s \in [0, 1]$
($\Leftarrow$)
Since $\nabla^2 f(x) \geq 0$, then

$$\frac{1}{2}(y - x)^T \nabla^2 f(x + s(y - x)) \cdot (y - x) \geq 0$$

Then

$$f(y) \geq f(x) + \nabla f(x) \cdot (y - x)$$

for all $x, y \in \Omega$.
Then by C^1 criterion, f is convex.
($\Rightarrow$)
Assume f is convex on Ω.
Suppose for contradiction that $\nabla^2 f(x)$ is not positive semi-definite at some $x \in \Omega$.
Then $\exists v \neq 0$ s.t. $v^T \nabla^2 f(x) v < 0$ v could be arbitrarily small and > 0
Let $y = x + v$, then

$$(y - x)^T \nabla^2 f(x + s(y - x)) \cdot (y - x) < 0$$

for all $s \in [0, 1]$
Then by MVT,

$$f(y) < f(x) + \nabla f(x) \cdot (y - x)$$

for some $x, y \in \Omega$, and this contradicts the C^1 criterion. ■

3.4 Minimization and Maximization of Convex Functions

Theorem f : convex $\Omega \subseteq \mathbb{R}^n \to \mathbb{R}$ is a convex function.
Suppose $\Gamma := \{x \in \Omega | f(x) = \min_{\Omega} f(x)\} \neq \emptyset$
(i.e. minimizer exists)
Then Γ is a convex set, and any local minimum of f is a global minimum of f.
proof:

Let $m = \min_{\Omega} f(x)$.

$$\Gamma = \{x \in \Omega | f(x) = m\} = \{x \in \Omega | f(x) \leq m\}$$

(sublevel set)
Then by Basic Properties of Convex Sets, Γ is convex.
Let x be a local minimum of f.
Suppose for contradiction that $\exists y$ s.t. $f(y) < f(x)$
(i.e. x is not a global minimum)

$$\begin{aligned} f(sy + (1 - s)x) &\leq sf(y) + (1 - s)f(x) \\ &< sf(x) + (1 - s)f(x) && (f(y) < f(x)) \\ &= f(x) \end{aligned}$$

for all $s \in (0, 1)$
As s approaches 0, s approaches x.
Then we have $\lim_{s \to 0} f(sy + (1 - s)x) = f(x) < f(x)$.
which is a contradiction. ■

Theorem If $f : \Omega \subseteq \mathbb{R}^n \to \mathbb{R}$ is a convex function, and Ω is convex and compact, then

$$\max_{\Omega} f = \max_{\partial\Omega} f$$

Remarks Maximum value of f is attained (also) on the boundary of Ω
proof:
Since Ω is closed, $\partial\Omega \subseteq \Omega$, so $\max_{\Omega} f \geq \max_{\partial\Omega} f$.
Suppose $f(x_0) = \max_{\Omega} f$ for some $x_0 \notin \partial\Omega$. Let L be an arbitrary line through x_0.

By convexity and compactness of Ω, L meets $\partial\Omega$ at two points x_1, x_2.
Let $x_0 + sx_1 + (1-s)x_2$ for $s \in (0,1)$

$$\begin{aligned} f(x_0) &= f(sx_1 + (1-s)x_2) \\ &\leq sf(x_1) + (1-s)f(x_2) && (f \text{ convex}) \\ &\leq \max\{f(x_1), f(x_2)\} \\ &\leq \max_{\partial\Omega} f \\ &\leq \max_{\Omega} f = f(x_0) \end{aligned}$$

This implies that

$$\max_{\Omega} f = \max_{\partial\Omega} f$$

as wanted. ■

Example

$$|ab| \leq \frac{1}{p}|a|^p + \frac{1}{q}|b|^q$$

where $p, q > 1$ s.t. $\frac{1}{p} + \frac{1}{q} = 1$.
Special cases:

1. $$p = q = 2, |ab| \leq \frac{|a|^2 + |b|^2}{2}$$

2. $$p = 3, q = \frac{3}{2}, |ab| \leq \frac{1}{3}|a|^3 + \frac{2}{3}|b|^{\frac{3}{2}}$$

proof:
Since function $f(x) = -\log(x)$ is convex, then

$$\begin{aligned} (-\log)|ab| &= (-\log)|a| + (-\log)|b| \\ &= \frac{1}{p}(-\log)|a|^p + \frac{1}{q}(-\log)|b|^q \\ &\geq (-\log)(\frac{1}{p}|a|^p + \frac{1}{q}|b|^q) \\ (-\log)|ab| &\geq (-\log)(\frac{1}{p}|a|^p + \frac{1}{q}|b|^q) \\ \log|ab| &\leq \log(\frac{1}{p}|a|^p + \frac{1}{q}|b|^q) \\ |ab| &\leq \frac{1}{p}|a|^p + \frac{1}{q}|b|^q && \text{(exponential function is increasing)} \end{aligned}$$

■

4 Basics of Unconstrained Optimization

4.1 Extreme Value Theorem

Suppose $f : \mathbb{R}^n \to \mathbb{R}$ is continuous, and compact set $K \subseteq \mathbb{R}^n$ Then the problem

$$\min_{x \in K} f(x)$$

has a solution.

Recall

1. $$K \subseteq \mathbb{R}^n \text{ compact } \iff K \text{ closed and bounded}$$

2. If $h_1, \ldots, h_k$ and $g_1, \ldots, g_m$ are continuous functions on $\mathbb{R}^n$, then the set of all points $x \in \mathbb{R}^n$ s.t.

$$\begin{cases} h_i(x) = 0 & \text{for all } i \\ g_j(x) \leq 0 & \text{for all } j \end{cases}$$

   is a closed set.

3. If such a set is also bounded, then it is compact.

Example

$$\{(x, y) \in \mathbb{R}^2 | x^2 + y^2 - 1 = 0\}$$

by (2), this is a closed set
by (3), this is a compact set.

Remarks $f : \Omega \subseteq \mathbb{R}^n \to \mathbb{R}$ convex does not imply f is continuous.

4.2 Unconstrained Optimization

$$\min_{x \in \Omega \subseteq \mathbb{R}^n} f(x)$$

typically

1. $\Omega \subseteq \mathbb{R}^n$
2. $\Omega = \mathbb{R}^n$
3. $\Omega =$ open
4. $\Omega = \overline{\text{open}}$

Remark

1. $\max f(x) = -(\min -f(x))$
2. $\min f(x) = -(\max -f(x))$

Definition: local minimum We say that f has a <u>local minimum</u> at a point $x_0 \in \Omega$ if

$$f(x_0) \leq f(x)$$

for all $x \in B^{\varepsilon}_{\Omega}(x_0)$, where $B^{\varepsilon}_{\Omega}(x_0) = \{x \in \Omega : |x - x_0| < \varepsilon\}$ which is an open ball around x_0 inside Ω of radius $\varepsilon > 0$.
We say that f has a <u>strict local minimum</u> at a point $x_0 \in \Omega$ if

$$f(x_0) < f(x)$$

for all $x \in B^{\varepsilon}_{\Omega}(x_0) \setminus \{x_0\}$

4.3 1st order necessary condition for local minimum

Theorem Let f be a C^1 function on $\Omega \subseteq \mathbb{R}^n$. If $x_0 \in \Omega$ is a local minimum of f, then

$$\nabla f(x_0) \cdot v \geq 0$$

for all feasible directions v at x_0

Definition: feasible direction $v \in \mathbb{R}^n$ is a feasible direction at $x_0 \in \Omega$ if

$$x_0 + sv \in \Omega$$

for all $0 \leq s \leq \bar{s}$ where $\bar{s} \in \mathbb{R}$

Remarks Feasible directions go into the set.

Corollary Special case: If $\Omega = \mathbb{R}^n$ is an open set, then any direction is a feasible direction. Then x_0 is a local minimum of f on Ω implies that $\nabla f(x_0) \cdot v \geq 0$ for all $v \in \mathbb{R}^n$.

$$\begin{cases} \nabla f(x_0) \cdot v \geq 0 \\ \nabla f(x_0) \cdot (-v) \geq 0 \iff \nabla f(x_0) \cdot v \leq 0 \end{cases} \implies \nabla f(x_0) \cdot v = 0 \text{ for all } v \in \mathbb{R}^n$$

$$\implies \nabla f(x_0) = 0$$

. ■

4.4 2nd order necessary condition for local minimum

$f \in C^2, \Omega \subseteq \mathbb{R}^n$
If $x_0 \in \Omega$ is a local minimum of f on Ω, then

1. $\nabla f(x_0) \cdot v \geq 0$ for al feasible directions v at x_0
2. If $\nabla f(x_0) \cdot v = 0$, then $v^T \nabla^2 f(x_0) v \geq 0$ (function curves up)

. ■

Remark If x_0 is an interior point of Ω, then

$$\nabla f(x_0) = 0, \quad \nabla^2 f(x_0) \geq 0$$

$$f'(x_0) = 0, \quad f''(x_0) \geq 0$$

Definition: principal minor Let A be an $n \times n$ matrix. A $k \times k$ submatrix of A formed by deleting $n-k$ rows of A, and the same $n-k$ columns of A, is called principal submatrix of A. The determinant of a principal submatrix of A is called a principal minor of A.

Definition: leading principal minor Let A be an $n \times n$ matrix. The kth order principal submatrix of A obtained by deleting the last $n-k$ rows and columns of A is called the k-th order leading principal submatrix of A, and its determinant is called a leading principal minor of A.

Definition: positive definiteness (Sylvester's Criterion) A $n \times n$ matrix A is

1. positive definite if $v^T A v > 0$ for all $v \neq 0 \iff$ all eigenvalues $> 0 \iff$ all leading principle minors > 0
2. positive semi-definite if $v^T A v \geq 0$ for all $v \iff$ all eigenvalues $\geq 0 \iff$ all principle minors ≥ 0

Lemma Suppose $\nabla^2 f(x_0)$ is positive definite, then

$$\exists a > 0 \ s.t. \ v^T \nabla^2 f(x_0) v \geq a||v||^2 \quad \forall v$$

4.5 2nd order sufficient condition (for interior points)

$f \in C^2$ on Ω

If $\begin{cases} \nabla f(x_0) = 0 \\ \nabla^2 f(x_0) > 0 \end{cases}$, then x_0 is a strict local minimum.

. ■

5 Optimization with Equality Constraints

5.1 Definitions of Related Spaces

Definition 5.1.1: surface

$$M = \text{“surface”} = \{x \in \mathbb{R}^n | h_1(x) = 0, \ldots, h_k(x) = 0\}$$

where $h_i \in C^1$

Definition 5.1.2: differentiable curve on surface A differentiable curve on surface $M \subseteq \mathbb{R}^n$ is a C^1 function

$$x : (-\epsilon, \epsilon) \to M : s \mapsto x(s)$$

Remarks

1. Let $x(s)$ be a differentiable curve on M that passes through $x_0 \in M$, say $x(0) = x_0$. The vector $v = \frac{d}{ds}|_{s=0} x(0)$ touches M “tangentially”. We say v is generated by $x(s)$.
2. In previous calculus courses, differentiable curves are often referred to as parameterizations.

Definition 5.1.3: tangent vector Any vector v which is generated by some differentiable curve on M through x_0 is called a tangent vector.

Definition 5.1.4: tangent space Tangent space to the surface M at point x_0 is

$$T_{x_0} M = \{\text{all tangent vectors to } M \text{ at } x_0\} = \{v \in \mathbb{R}^n : v = \frac{d}{ds}|_{s=0} x(s)\}$$

where $x(s)$ is a differentiable curve on M s.t. $x(0) = x_0$

Remarks The zero vector is contained in all tangent spaces.

Definition 5.1.5: T-space

$$T_{x_0} = \{x \in \mathbb{R}^n : x^T \nabla h_i(x_0) = 0 \, \forall i\} = Span\{\nabla h_1(x_0), \ldots, \nabla h_k(x_0)\}^\perp$$

Definition 5.1.6: regular point $x_0 \in M$ is a regular point (of the constraints) if $\{\nabla h_1(x_0), \ldots . \nabla h_k(x_0)\}$ are linearly independent.

Remark If there is only one constraint h, then x_0 is regular if and only if $\nabla h(x_0) \neq 0$.

When does the T-space equivalent to the tangent space? When x_0 is a regular point (of the constraints).

Theorem 5.1.7 Suppose x_0 is a regular point s.t. $M = \{x \in \mathbb{R}^n : h_i(x) = 0 \, \forall i\}$. Then

$$T_{x_0} M = T_{x_0}$$

Lemma 5.1.8 $f, h_1, \ldots, h_k \in C^1$ on open $\Omega \subseteq \mathbb{R}^n$
$M = \{x \in \mathbb{R}^n : h_i(x) = 0 \, \forall i\}$
Suppose $x_0 \in M$ is a local minimum of f on M, then

$$\nabla f(x_0) \perp T_{x_0} M \iff \nabla f(x_0) \cdot v = 0$$

for all $v \in T_{x_0} M$

5.2 Lagrange Multipliers: 1st order necessary condition for local minimum

$f, h_1, \ldots, h_k \in C^1$ on open $\Omega \subseteq \mathbb{R}^n$.
Let x_0 be a regular point of the constraints $M = \{x \in \mathbb{R}^n : h_i(x) = 0 \, \forall i\}$.
Suppose x_0 is a local minimum of f on M, then $\exists \lambda_1, \ldots, \lambda_k \in \mathbb{R}$ s.t.

$$\nabla f(x_0) + \lambda_1 \nabla h_1(x_0) + \ldots + \lambda_k \nabla h_k(x_0) = 0$$

Proof. x_0 regular implies that

$$T_{x_0} M = T_{x_0} = Span\{\nabla h_1(x_0), \ldots, \nabla h_k(x_0)\}^{\perp}$$

By Lemma 5.1.8, x_0 is a loc min implies that

$$\nabla f(x_0) \perp T_{x_0} M$$

Then

$$\nabla f(x_0) \in (T_{x_0} M)^{\perp} = Span\{\nabla h_i(x_0)\}^{\perp\perp} = Span\{\nabla h_i(x_0)\}$$

Then

$$\nabla f(x_0) = -\lambda_1 \nabla h_1(x_0) - \ldots - \lambda_k \nabla h_k(x_0)$$

for some $\lambda_i \in \mathbb{R}$ ■

5.3 2nd order necessary condition for local minimum

$f, h_1, \ldots, h_k \in C^2$ on open $\Omega \subseteq \mathbb{R}^n$.
Let x_0 be a regular point of the constraints $M = \{x \in \mathbb{R}^n : h_i(x) = 0 \, \forall i\}$.
Suppose x_0 is a local minimum of f on M, then

1. $$\nabla f(x_0) + \sum_{i=1}^{k} \lambda_i \nabla h_i(x_0) = 0$$

   for some $\lambda_i \in \mathbb{R}$

2. $$\nabla^2 f(x_0) + \sum \lambda_i \nabla^2 h_i(x_0) \geq 0$$

   on $T_{x_0} M$

5.4 2nd order sufficient condition for local minimum

$f, h_1, \dots, h_k \in C^2$ on open $\Omega \subseteq \mathbb{R}^n$.
Let x_0 be a regular point of the constraints $M = \{x \in \mathbb{R}^n : h_i(x) = 0 \, \forall i\}$.
If $\exists \lambda_i \in \mathbb{R}$ s.t.

1. $$\nabla f(x_0) + \sum \lambda_i \nabla h_i(x_0) = 0$$
2. $$\nabla^2 f(x_0) + \sum \lambda_i \nabla^2 h_i(x_0) > 0$$
   on $T_{x_0} M$

Then x_0 is a strict local minimum.

Proof. Recall that (2) means $[\nabla^2 f(x_0) + \sum \lambda_i h_i(x_0)]$ is pos-def on $T_{x_0} M$.
Then $\exists a > 0$ s.t. $v^T [\nabla^2 f(x_0) + \sum \lambda_i h_i(x_0)] v \geq a||v||^2$ for all $v \in T_{x_0} M$.
Let $x(s) \in M$ be a curve s.t. $x(0) = x_0$ and $v = x'(0)$.
WLOG, $||x'(0)|| = 1$.
By 2nd order Taylor,

$$\begin{aligned}
f(x(s)) - f(x(0)) &= s \frac{d}{ds}|_{s=0} f(x(s)) + \frac{1}{2} s^2 \frac{d}{ds^2}|_{s=0} f(x(s)) + o(s^2) \\
&= s \frac{d}{ds}|_{s=0} [f(x(s)) + \sum_i \lambda_i h_i(x(s))] + \frac{1}{2} s^2 \frac{d}{ds^2}|_{s=0} [f(x(s)) + \sum_i \lambda_i h_i(x(s))] + o(s^2) \\
&\qquad\qquad (\textstyle\sum_i \lambda_i h_i(x(s)) = 0) \\
&= s[\nabla f(x_0) + \sum \lambda_i \nabla h_i(x_0)] \cdot x'(0) + \frac{1}{2} s^2 x'(0)^T [\nabla^2 f(x_0) + \sum \lambda_i \nabla^2 h_i(x_0)] x'(0) + o(s^2) \\
&= 0 + \frac{1}{2} s^2 v^T [\nabla^2 f(x_0) + \sum \lambda_i \nabla^2 h_i(x_0)] v + o(s^2) \\
&\geq \frac{1}{2} s^2 a ||v||^2 + o(s^2) \\
&= \frac{1}{2} s^2 a + o(s^2) \\
&= s^2 [\frac{a}{2} + \frac{o(s^2)}{s^2}] > 0
\end{aligned}$$

for small $s > 0$, since $\frac{a}{2} > 0$ and $\lim_{s \to 0} \frac{o(s^2)}{s^2} = 0$
Then $f(x(s)) > f(x_0)$ for small $s > 0$ Then x_0 is a strict local min of f. ■

6 Optimization with Inequality Constraints

Problem open $\Omega \subseteq \mathbb{R}^n$
$f : \Omega \to \mathbb{R}$
$h_1, \dots, h_k : \Omega \to \mathbb{R}$
$g_1, \dots, g_l : \Omega \to \mathbb{R}$

$$\begin{cases} \min f(x) \\ x \in \Omega \text{ subject to } \begin{cases} h_1(x) = 0, \dots, h_k(x) = 0 \\ g_1(x) \leq 0, \dots, g_l(x) \leq 0 \end{cases} \end{cases} \qquad (*)$$

Definition 1: activeness Let x_0 satisfy the constraints.
We say that the constraint $g_i(x) \leq 0$ is active at x_0 if $g_i(x_0) = 0$.
It is inactive at x_0 if $g_i(x_0) < 0$.

Definition 2: regular point Suppose for some $l' \leq l$:

$$g_1(x) \leq 0, \ldots, g_{l'}(x) \leq 0;\ g_{l'+1}(x) \leq 0, \ldots, g_l(x) \leq 0$$

where $g_1, \ldots g_{l'}$ active and the rest inactive.
We say that x_0 is a regular point of the constraints if
$\{\nabla h_1(x_0), \ldots, \nabla h_k(x_0), \nabla g_1(x_0), \ldots, \nabla g_{l'}(x_0)\}$ is linearly independent.

6.1 Kuhn-Tucker conditions: 1st order necessary condition for local minimum

open $\Omega \subseteq \mathbb{R}^n$
$f : \Omega \to \mathbb{R}$
$h_1, \ldots, h_k, g_1, \ldots, g_l : C^1 \in \Omega$
Suppose $x_0 \in \Omega$ is a regular point of the constraints which is a local minimum, then

1. $$\nabla f(x_0) + \sum_{i=1}^{k} \lambda_i \nabla h_i(x_0) + \sum_{j=1}^{l} \mu_j \nabla g_j(x_0) = 0$$

   for some $\lambda_i \in \mathbb{R}$ and $\mu_j \geq 0$

2. $\mu_j g_j(x_0) = 0$

Remark 1 Given x_0,

$$\begin{cases} g_j(x) \leq 0 \text{ active at } x_0 \implies g_j(x_0) = 0 \implies \mu_j g_j(x_0) = 0 \\ g_j(x) \leq 0 \text{ inactive at } x_0 \implies g_j(x_0) < 0 \implies \mu_j = 0 \end{cases}$$

$\implies \mu_j = 0$ for all inactive g_j at x_0

Remark 2 It is possible for an active constraint to have zero multiplier.

Remark 3 $\mu_j \geq 0$ because ∇f and ∇g have opposite directions at a local minimum x_0.

$$\nabla f(x_0) + \mu \nabla g(x_0) = 0 \implies \nabla f(x_0) = -\mu \nabla g(x_0) \implies -\mu < 0 \implies \mu > 0$$

Is this true?

Idea of proof x_0 is a local min of f subject to (*)
$\implies$ x_0 is a local min for equality constraints $h_1(x) = 0, \ldots, h_k(x) = 0$+ active inequality constraints $g_1(x) \leq 0, \ldots, g_{l'}(x) \leq 0$
$\implies$ x_0 is a local min for $h_1(x) = 0, \ldots, h_k(x) = 0 + g_1(x) = 0, \ldots, g_{l'}(x) = 0 \implies \nabla f(x_0) + \sum_{i=1}^{k} \lambda_i \nabla h_i(x_0) + \sum_{j=1}^{l'} \mu_j \nabla g_j(x_0) = 0$
for some $\lambda_i \in \mathbb{R}$ and $\mu_j \in \mathbb{R}$.
Let $\mu_j = 0$ for $j = l' + 1, \ldots, l$, then

$$\nabla f(x_0) + \sum_{i=1}^{k} \lambda_i \nabla h_i(x_0) + \sum_{j=1}^{l} \mu_j \nabla g_j(x_0) = 0$$

6.2 2nd order necessary conditions for local minimum

Open $\Omega \subseteq \mathbb{R}^n$, $f, h_1, \ldots, h_k, g_1, \ldots, g_l \in C^2$. Let x_0 be a regular point of the constraints:

$$(\dagger) \begin{cases} h_1(x) = \ldots = h_k(x_0) = 0 \\ g_1(x), \ldots g_l(x_0) \leq 0 \end{cases}$$

Suppose x_0 is a local min of f subject to $(\dagger)$. Then, $\exists \lambda_i \in \mathbb{R}, \mu_j \geq 0$ s.t.

1. $\nabla f(x_0) + \sum_{i=1}^k \lambda_i \nabla h_i(x_0) + \sum_{j=1}^l \mu_j \nabla g_j(x_0) = 0$
2. $\mu_j g_j(x_0) = 0$ for all j
3. $[\nabla^2 f(x_0) + \sum \lambda_i \nabla^2 h_i(x_0) + \sum \mu_j \nabla^2 g_h(x_0)]]$ is positive semi definite on tangent space to active constraints at x_0.

Proof. x_0 local min for $(\dagger)$
$\implies$ x_0 local min for only active constraints at x_0.
$\implies \begin{cases} h_i(x) = 0 \ \forall i \\ g_j(x) = 0 \ j = 1, \ldots, l' \end{cases}$
$\implies$ $[\nabla^2 f(x_0) + \sum \lambda_i \nabla^2 h_i(x_0) + \sum \mu_j \nabla^2 g_h(x_0)]$ pos semi def on tangent space to active constraints. ■

6.3 2nd order sufficient conditions

Open $\Omega \subseteq \mathbb{R}^n$, $f, h_i, g_j \in C^2$ on Ω.
Problem:

$$\begin{cases} \min & f(x) \\ \text{subject to} & \begin{cases} h_i(x) = 0 \\ g_j(x) \leq 0 \end{cases} \end{cases}$$

Suppose $\exists x_0$ feasible and $\lambda_i, \mu_j \in \mathbb{R}$ s.t.

1. $\nabla f(x_0) + \sum_{i=1}^k \lambda_i \nabla h_i(x) + \sum_{j=1}^l \mu_j \nabla g_j(x_0) = 0$
2. $\mu_j g_j(x_0) = 0$ all j

If the Hessian matrix, $L(x_0) = \nabla^2 f(x_0) + \sum_{i=1}^k \lambda_i \nabla^2 f(x_0) + \sum_{i=1}^l \mu_j \nabla^2 g_j(x)$ is pos def on $\tilde{\tilde{T}}_{x_0}$-space of "strongly active" constraints at x_0.
Then x_0 is a strict local min.

Remarks

1. $$\text{Active constraints at } x_0 \begin{cases} h_i(x) = 0 & i = 1, \ldots, k \\ g_j(x) \leq 0 & j = 1, \ldots, l' \end{cases} \implies g_j(x_0) = 0$$

2. $$\text{Strongly active constraints at } x_0 \begin{cases} h_i(x) = 0 & i = 1, \ldots, k \\ g_j(x) \leq 0 & j = 1, \ldots, l'' \end{cases} g_j(x) \text{ is active at } x_0 \text{ and } \mu_j > 0$$

   $l'' \leq l' \leq l$

3. $$\tilde{\tilde{T}}_{x_0} = \{v \in \mathbb{R}^n | v \cdot \nabla h_i(x_0) = 0 \text{ all } i \text{ and } v \cdot \nabla g_j(x_0) = 0 \text{ for all } j = 1, \ldots, l''\}$$

4. strongly active $\subseteq$ active
   $\implies \tilde{\tilde{T}}_{x_0} = (\text{strongly active})^{\perp} \supseteq (\text{active})^{\perp} = \tilde{T}_{x_0}$

Proof. (details see another pdf by prof) Suppose x_0 is NOT a (strict) local min.
claim: $\exists$ unit vector $v \in \mathbb{R}$ s.t.

1. $\nabla f(x_0) \cdot v \leq 0$
2. $\nabla h_i(x_0) \cdot v = 0 \quad i = 1, \ldots, k$
3. $\nabla g_j(x_0) \cdot v \leq 0 \quad j = 1, \ldots, l'$

proof of claim: []
claim: $\nabla g_j(x) \cdot v = 0$ for $j = 1, \ldots, l''$
proof of claim: []
$\implies$ contradiction!
claim: $\exists$ unit vector $v \in \mathbb{R}$ s.t.

1. $\nabla f(x_0) \cdot v \leq 0$
2. $\nabla h_i(x_0) \cdot v = 0 \quad i = 1, \ldots, k$
3. $\nabla g_j(x_0) \cdot v = 0 \quad j = 1, \ldots, l''$

proof of claim: [] ■

7 Different Computation Methods for Solving Optimum

7.1 Newton's Method

$x_0 \in I$ start
$x_{n+1} = x_0 - \frac{f'(x_0)}{f''(x_0)}$

Theorem Let $f \in C^3$ on I.
Suppose $x_* \in I$ satisfies $f'(x_*) = 0$ and $f''(x_*) \neq 0$ (x_* is a non-degenerate (non-singular) critical point).
Then the sequence of points $\{x_n\}$ generated by Newton's method

$$x_{n+1} = x_n - \frac{f'(x_0)}{f''(x_0)}$$

converges to x_* if x_0 is sufficiently close to x_*.

Why do we need this method? In real life, we may not know the real function formula. We only have data, using which we can approximate the function formula. In a way, Newton's method is true "applied mathematics".

Proof of Theorem Let $g(x) = f'(x)$ so that $x_{n+1} = x_n - \frac{g(x_n)}{g'(x_n)}$
By $g \in C^2, \exists \alpha$ s.t. $|g'(x_1)| > \alpha \, \forall x_1$ and $|g''(x_2)| < \frac{1}{\alpha} \; \forall x_2$ in a neighbourhood of x_* (choose α small enough).

$$x_{n+1} - x_* = x_n - \frac{g(x_n)}{g'(x_n)} - x_* \tag{1}$$
$$= x_n - x_* - \frac{g(x_n) - g(x_*)}{g'(x_n)} \qquad (g(x_*) = 0) \tag{2}$$
$$= \frac{-[g(x_n) - g(x_*) - g'(x_n)(x_n - x_*)]}{g'(x_n)} \tag{3}$$
$$= \frac{1}{2}\frac{g''(\xi)}{g'(x_n)}(x_n - x_*)^2 \tag{4}$$
$$|x_{n+1} - x_*| = \frac{1}{2}\frac{g''(\xi)}{g'(x_n)}|x_n - x_*|^2 < \frac{1}{2\alpha^2}|x_n - x_*|^2 \qquad \text{(in small neighbourhood of } x_*) \tag{5}$$
$$\rho := \frac{1}{2\alpha^2}|x_0 - x_*| \qquad \text{(choose } x_0 \text{ sufficiently close to } x_* \text{ s.t. } \rho < 1) \tag{6}$$
$$|x_1 - x_*| < \frac{1}{2\alpha^2}|x_0 - x_*|^2 \tag{7}$$
$$= \frac{1}{2\alpha^2}|x_0 - x_*||x_0 - x_*| \tag{8}$$
$$= \rho|x_0 - x_*| \tag{9}$$
$$|x_2 - x_*| < \frac{1}{2\alpha^2}|x_1 - x_*|^2 \tag{10}$$
$$< \frac{1}{2\alpha^2}\rho^2|x_0 - x_*|^2 \tag{11}$$
$$= \frac{1}{2\alpha^2}|x_0 - x_*|\rho^2|x_0 - x_*| \tag{12}$$
$$< \rho^2|x_0 - x_*| \qquad (\rho < 1) \tag{13}$$
$$|x_n - x_*| < \rho^n|x_0 - x_*| \underset{n\to\infty}{\to} 0 \tag{14}$$
$$\implies x_n \to x_* \tag{15}$$

proof of (4):
By 2nd order MVT,

$$g(x) = g(y) + g'(y)(x - y) + \frac{1}{2}g''(\xi)(x - y)^2$$

for some $\xi \in [x, y]$.
Let $x = x_*$ and $y = x_n$, then

$$g(x_*) = g(x_n) + g'(x_n)(x_* - x_n) + \frac{1}{2}g''(\xi)(x_* - x_n)^2$$

$$\implies -[g(x_n) - g(x_*) - g'(x_n)(x_n - x_*)] = \frac{1}{2}g''(\xi)(x_n - x_*)^2$$

■

Newton's Method (generalized) $f : \Omega \underset{open}{\subseteq} \mathbb{R}^n \to \mathbb{R}$ and $f \in C^3$ on Ω
$x_0 \in \Omega$
$x_{n+1} = x_n - [\nabla^2 f(x_n)]^{-1}\nabla f(x_n)$
(The algorithm requires $\nabla^2 f(x_n)$ invertible and stops when $\nabla f(x_n) = 0$)

Note Newton's method may fail to converge even if $f(x)$ has a unique global min x_* and x_0 is arbitrarily close to x_*

Remark Newton's method, if converge, converges to

1. local min
2. local max
3. saddle point

Example 7.1. Newton's Method on Quadratic Function Let Q be a symmetric $n \times n$ invertible matrix. Define quadratic form $f(x) := \frac{1}{2}x^T Qx : \mathbb{R}^n \to \mathbb{R}$. Then the optima is $x = 0$.
Let $x_0 \in \mathbb{R}^n$, then

$$x_1 := x_0 - \nabla^2 f(x_0)^{-1} \nabla f(x_0) = x_0 - Q^{-1}Qx_0 = 0$$

Newton's method converges in one iteration.

7.2 Method of Steepest Descent (Gradient Method)

$f : \Omega \underset{open}{\subseteq} \mathbb{R}^n \to \mathbb{R}, C^1$
Recall: Direction of steepest ascent at x_0 is given by the direction of gradient $\nabla f(x_0)$

Algorithm of steepest descent $x_0 \in \Omega$

$$x_{k+1} = x_k - \alpha_k \nabla f(x_k)$$

where $\alpha_k \geq 0$ satisfying $f(x_k - \alpha_k \nabla f(x_k)) = \min_{\alpha \geq 0} f(x_k - \alpha \nabla f(x_k))$
(keep going until you find the minimum)

Fact: algorithm is descending If $\nabla f(x_k) \neq 0$, then $f(x_{k+1}) < f(x_k)$
Why? $f(x_{k+1}) = f(x_k - \alpha_k \nabla f(x_k)) \leq f(x_k - \alpha \nabla f(x_k))$ for all $0 < \alpha \leq \alpha_k$
Recall: $\frac{d}{ds}|_{s=0} f(x_k - s\nabla f(x_k)) = \nabla f(x_k) \cdot (-\nabla f(x_k)) = -|\nabla f(x_k)|^2 < 0$
$\implies f(x_{k+1}) \leq f(x_k - \alpha \nabla f(x_k)) < f(x_k)$ for small α

Fact: the method of steepest descent moves perpendicular steps

$$(x_{k+2} - x_{k+1}) \cdot (x_{k+1} - x_k) = (-\alpha_{k+1} \nabla f(x_{k+1})) \cdot (-\alpha_k \nabla f(x_k)) \tag{16}$$
$$= \alpha_k \alpha_{k+1} \nabla f(x_{k+1}) \cdot \nabla f(x_k) \tag{17}$$
$$\tag{18}$$

If $\alpha_k = 0$, then we are done.
If $\alpha_k \neq 0$, then

$$\nabla f(x_{k+1}) = \min_{\alpha \geq 0} f(x_k - \alpha \nabla f(x_k)) \tag{19}$$
$$\implies \frac{d}{d\alpha}|_{\alpha = \alpha_k} f(x_k - \alpha \nabla f(x_k)) = (-\nabla f(x_k)) \cdot \nabla f(x_k - \alpha_k \nabla f(x_k)) = 0 \tag{20}$$
$$\implies \alpha_k \alpha_{k+1} \nabla f(x_{k+1}) \cdot \nabla f(x_k) = 0 \tag{21}$$

Note This method is not the most efficient. May take infinite steps to converge.

Theorem (Convergence of Steepest Descent) $f \in C^1$ on $\Omega \underset{open}{\subseteq} \mathbb{R}^n$

Let $\{x_k\}$ be sequence generated by steepest descent.
$x_{k+1} = x_k - \alpha_k \nabla f(x_k)$
If $\{x_k\}$ is "bounded in Ω" (i.e. $\exists$ compact set $K \subset \Omega$ s.t. $x_k \in K$ for all k)
Then every convergent subsequence of $\{x_k\}$ converges to a critical point $x_* \in \Omega$ of $f : \nabla f(x_*) = 0$

Proof. $x_k \in$ compact $K \implies$ subsequence $x_{k_i} \to x_* \in K$
Since $f(x_0) \geq f(x_1) \geq f(x_2) \geq \ldots$ and $f(x_{k_i}) \searrow f(x_*)$
Suppose by contradiction that $\nabla f(x_*) \neq 0$
$x_{k_i} \to x_* \implies \nabla f(x_{k_i}) \to \nabla f(x_*)$
Let $y_{k_i} = x_{k_i} - \alpha_{k_i} \nabla f(x_{k_i}) = x_{k_i+1}$. Then $y_{k_i} \to y_*$. Then

$$f(y_{k_i}) = f(x_{k_i+1}) = \min_{\alpha \geq 0} f(x_i - \alpha \nabla f(x_{k_i})) \tag{22}$$
$$f(y_{k_i}) \leq f(x_{k_i} - \alpha \nabla f(x_{k_i})) \text{ for all } \alpha \geq 0 \tag{23}$$
$$\lim_{i \to \infty} f(y_*) \leq f(x_* - \alpha \nabla f(x_*)) \text{ for all } \alpha \geq 0 \tag{24}$$
$$f(y_*) \leq \min_{\alpha \geq 0} f(x_* - \alpha \nabla f(x_*)) < f(x_*) \tag{25}$$
$$f(y_*) < f(x_*) \tag{26}$$
$$\tag{27}$$

But $f(y_*) = \lim_{i \to \infty} f(y_{k_i}) = \lim_{i \to \infty} f(x_{k_i+1}) = f(x_*)$, so we have a contradiction. ■

Steepest descent: Quadratic case Let f follow the general quadratic form

$$f(x) = \frac{1}{2} x^T Q x - b^T x$$

where $b, x \in \mathbb{R}^n$ and Q is an $n \times n$ positive definite matrix.
Let $0 < \lambda = \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n = \Lambda$ be eigenvalues of Q.
Recall that if Q pos-def, then there is a unique minimum x_* such that $Qx_* - b = 0 \iff x_* = Q^{-1} b$
Define $q(x) := \frac{1}{2}(x - x^*)^T Q (x - x^*) = f(x) + const$
Note that $q(x) \geq 0$ and $q(x_*) = 0$.
Define $g(x) := Qx - b = \nabla q(x) = \nabla f(x)$
So using the method of steepest descent:

$$x_{k+1} = x_k - \alpha_k g(x_k)$$

Derive the formula for α_k:
α_k minimizes $f(x_k - \alpha g(x_k))$

$$0 = \frac{d}{d\alpha}|_{\alpha = \alpha_k} f(x_k - \alpha g(x_k)) \tag{28}$$
$$= \nabla f(x_k - \alpha_k g(x_k)) \cdot (-g(x_k)) \tag{29}$$
$$= -[Q(x_k - \alpha_k g(x_k)) - b] \cdot (g(x_k)) \tag{30}$$
$$= -(Qx_k - b) \cdot g(x_k) \tag{31}$$
$$= -|g(x_k)|^2 + \alpha_k g(x_k)^T Q g(x_k) \tag{32}$$
$$\implies \alpha_k = \frac{|g(x_k)|^2}{g(x_k)^T Q g(x_k)} \tag{33}$$
$$\implies x_{k+1} = x_k - \alpha_k g(x_k) \tag{34}$$
$$= x_k - \frac{|g(x_k)|^2}{g(x_k)^T Q g(x_k)} g(x_k) \tag{35}$$

Claim:

$$q(x_{k+1}) = \left(1 - \frac{|g(x_k)|^4}{(g(x_k)^T Q g(x_k))(g(x_k)^T Q^{-1} g(x_k))}\right) g(x_k)$$

Proof.

$$\begin{aligned}
q(x_{k+1}) &= q(x_k - \alpha_k g(x_k)) && (36)\\
&= \frac{1}{2}(x_k - \alpha_k g(x_k) - x_*)^T Q (x_k - \alpha_k g(x_k) - x_*) && (37)\\
&= \frac{1}{2}(x_k - x_* - \alpha_k g(x_k))^T Q ((x_k - x_*) - \alpha_k g(x_k)) && (38)\\
&= \frac{1}{2}(x_k - x_*)^T Q (x_k - x_*) - \alpha_k g(x_k)^T Q (x_k - x_*) + \frac{1}{2}\alpha_k^2 g(x_k)^T Q g(x_k) && (39)\\
&= q(x_k) - \alpha_k g(x_k)^T Q (x_k - x_*) + \frac{1}{2}\alpha_k^2 g(x_k)^T Q g(x_k) && (40)\\
\implies q(x_k) - q(x_{k+1}) &= -\frac{1}{2}\alpha_k^2 g(x_k)^T Q g(x_k) + \alpha_k g(x_k)^T Q (x_k - x_*) && (41)\\
y_k &:= x_k - x_* && (42)\\
\frac{q(x_k) - q(x_{k+1})}{q(x_k)} &= \frac{-\frac{1}{2}\alpha_k^2 g(x_k)^T Q g(x_k) + \alpha_k g(x_k)^T Q y_k}{\frac{1}{2} y_k^T Q y_k} && (43)\\
&= \frac{2\alpha_k g(x_k)^T Q y_k - \alpha_k^2 g(x_k)^T Q g(x_k)}{y_k^T Q y_k} && (44)\\
&\quad (g_k := g(x_k) = Qx_k - b = Qx_k - Qx_* = Q(x_k - x_*) = Qy_k \implies y_k = Q^{-1} g_k) && (45)\\
&= \frac{2\alpha_k |g_k|^2 - \alpha_k^2 g_k^T Q g_k}{g_k^T Q^{-1} g_k} && (46)\\
&= \frac{2\frac{|g_k|^4}{g_k^T Q g_k} - \frac{|g_k|^4}{g_k^T Q g_k}}{g_k^T Q^{-1} g_k} && (47)\\
&= \frac{|g_k|^4}{(g_k^T Q g_k)(g_k^T Q^{-1} g_k)} && (\alpha_k = \tfrac{|g(x_k)|^2}{g(x_k)^T Q g(x_k)})\\
\implies q(x_k) - q(x_{k+1}) &= \left(\frac{|g_k|^4}{(g_k^T Q g_k)(g_k^T Q^{-1} g_k)}\right) q(x_k) && (48)\\
\implies q(x_{k+1}) &= q(x_k)\left(1 - \frac{|g_k|^4}{(g_k^T Q g_k)(g_k^T Q^{-1} g_k)}\right) && (49)\\
&\leq (1 - \frac{4\lambda\Lambda}{(\lambda+\Lambda)^2}) q(x_k) && \text{(By Kantorovich Inequality)}\\
\implies q(x_{k+1}) &\leq \frac{(\Lambda - \lambda)^2}{(\lambda + \Lambda)^2} q(x_k) && (50)
\end{aligned}$$

■

Kantorovich Inequality $Q : n \times n$ positive definite symmetric matrix
$\lambda = \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n = \Lambda$
For any $v \in \mathbb{R}^n$:

$$\frac{|v|^4}{(v^T Q v)(v^T Q^{-1} v)} \geq \frac{4\lambda\Lambda}{(\lambda + \Lambda)^2}$$

Theorem: Steepest Descent in Quadratic Case For any $x_0 \in \mathbb{R}^n$, method of steepest descent converges to the unique min point x_* of f.

Furthermore, for $q(x) := \frac{1}{2}(x-x_*)Q(x-x_*)$, where Q symmetric positive definite and $0 < \lambda = \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n = \Lambda$,

$$q(x_{k+1}) \leq \frac{(\Lambda-\lambda)^2}{(\lambda+\Lambda)^2} q(x_k)$$

Let $r := \frac{(\Lambda-\lambda)^2}{(\lambda+\Lambda)^2}$, then

$$q(x_k) \leq r^k q(x_0)$$

for all k. As $k \to \infty$, $q(x_k) \to 0$.

Notes

1. $x_k \in \{x \in \mathbb{R}^n | q(x) \leq r^k q(x_0)\} = SL_k$
   (sublevel set of function $q(x)$)
   Note that SL_k is strictly decreasing. Furthermore, note that x_* is the only point satisfying the inequality at the limit:
   $$q(x_*) = 0 = \lim_{k\to\infty} q(x_0)$$
   Therefore, $\lim_{k\to\infty} SL_k = \{0\}$, and $x_k \to x_*$.

2. $r = (\frac{(\Lambda-\lambda)}{(\lambda+\Lambda)})^2 = (\frac{\Lambda/\lambda-1}{\Lambda/\lambda+1})^2$ depends only on the ratio $\frac{\Lambda}{\lambda}$ = "condition number of Q"
   case $\frac{\Lambda}{\lambda} = 1 \implies r = 0 \implies 0 \leq q(x_1) \leq 0 \cdot q(x_0) \implies q(x_1) = 0 \implies x_1 = x_*$
   (Gradient descent converges to the unique global minimum in only one iteration.)
   case $\frac{\Lambda}{\lambda} >> 1 \implies r \simeq 1$
   (worst case, converges very flow)

7.3 Method of Conjugate Direction

Motivation Method of conjugate directions is designed for quadratic functions with form $f(x) = \frac{1}{2}x^TQx - b^Tx$. For other functional forms, one can approximate the function using quadratic form firstly and then apply method of conjugate directions.

Definition: Q-orthogonality Let Q be a symmetric matrix. Two vectors $d, d' \in \mathbb{R}^n$ are Q-orthogonal (or Q-conjugate) if

$$d^TQd' = 0$$

A finite set of $d_0, \ldots, d_k$ is called Q-orthogonal set if $d_i^TQd_j = 0$ for all $i \neq j$.

Example 1 Q is an identity matrix. d, d' are Q-orthogonal iff they are orthogonal.

Example 2 If d, d' are two eigenvectors with different eigenvalues, then they are Q-orthogonal.

Proof. Suppose $Qv = \lambda v$ and $Qw = \lambda' w$ so $\lambda \neq \lambda'$

$$< v, Qw > =< v, \lambda' w >= \lambda' < v, w > \tag{51}$$
$$=< Q^Tv, w >=< Qv, w >=< \lambda v, w >= \lambda < v, w > \tag{52}$$
$$\implies (\lambda - \lambda')\langle v, w\rangle = 0 \tag{53}$$

Since $(\lambda - \lambda') \neq 0$, them we have $\langle v, w\rangle = 0$.

$$\implies v^TQw = \langle v, Qw\rangle = \lambda\langle v, w\rangle = 0$$

■

Example 3 If Q is an $n \times n$ symmetric matrix, then there exists an orthogonal basis of eigenvectors $d_0, \ldots, d_{n-1}$
Claim: They are also Q-orthogonal.

Proof. $d_i^T Q d_j = d_i^T (\lambda d_j) = \lambda d_i^T d_j = 0$ ■

Proposition Let Q be a symmetric positive definite matrix. Let $d_0, \ldots, d_k$ be a set of (non-zero) Q-orthogonal vectors. Then $d_0, \ldots, d_k$ are linearly independent.

Proof. Assume $\alpha_0 d_0 + \ldots + \alpha_k d_k = 0$ for $\alpha_i \in \mathbb{R}$.
Multiply the whole equation by $d_i^T Q$:

$$\alpha_0 \underbrace{d_i^T Q d_0}_{=0} + \ldots + \alpha_i \underbrace{d_i^T Q d_i}_{>0} + \ldots + \alpha_k \underbrace{d_i^T Q d_k}_{=0} = 0$$

which implies $\alpha_i d_i^T Q d_i = 0$ and $\alpha_i = 0$.
This is true for every i. Therefore $d_0, \ldots, d_k$ are linearly independent. ■

Lemma (Theorems covered so far)

1. d_i, d_j are Q-orthogonal if $d_i^T Q d_j = 0$;
2. Eigen-vectors with different eigenvalues are Q-orthogonal;
3. Matrix Q symmetric $\implies$ there exists an orthogonal basis $\implies$ the set of basis is Q-orthogonal as well;
4. Q-orthogonal vectors are linearly independent.

Example 4 (Special case: Method of Conjugate Direction on Quadratic Functions). Let Q be a positive definite symmetric $n \times n$ matrix. The problem is

$$\min f(x) = \frac{1}{2} x^T Q x - b^T x$$

Recall that the unique global minimum is $x^* = Q^{-1} b$.
Let $d_0, d_1, \ldots, d_{n-1}$ be non-zero Q-orthogonal vectors.
Note that they are linearly independent by the previous theorem.
Therefore, they form a basis of $\mathbb{R}^n$.
The global minimum can be represented as

$$x^* = \sum_{j=0}^{n-1} \alpha_j d_j \, \alpha_j \in \mathbb{R}$$

For every j, the following holds:

$$d^T Q x^* = \alpha_j d_j^T Q d_j$$
$$\implies \alpha_j = \frac{d_j^T Q x^*}{d_j^T Q d_j}$$

Algorithm: Method of Conjugate Directions Let Q be a positive definite symmetric $n \times n$ matrix. and $\{d_j\}_{j=0}^{n-1}$ be a set of non-zero Q-orthogonal vectors, note that they form a basis of $\mathbb{R}^n$.
Given initial point $x_0 \in \mathbb{R}^n$, the method of conjugate direction generates a sequence of points $\{x_k\}_{k=0}^{n}$ as the following:

$$x_{k+1} \leftarrow x_k + \alpha_k d_k$$
$$\alpha_k := -\frac{\langle g_k, d_k \rangle}{d_k^T Q d_k} \; g_k := \nabla f(x_k)$$

Theorem Given the method of conjugate, the sequence of points generated eventually reaches the global minimum. That is, $x_n = x^*$.

Proof. Let $x^*, x_0 \in \mathbb{R}^n$, consider

$$x^* - x_0 = \sum_{j=0}^{n-1} \beta_j d_j \tag{54}$$

$$\iff x^* = x_0 + \sum_{j=0}^{n-1} \beta_j d_j \tag{55}$$

$$d_j^T Q(x^* - x_0 = d_j^T Q(\sum_{j=0}^{n-1} \beta_j d_j) \tag{56}$$

$$= \beta_j d_j^T Q d_j \tag{57}$$

$$\implies \beta_j = \frac{d_j^T Q(x^* - x_0)}{d_j^T Q d_j} \tag{58}$$

Note that the algorithm generates the sequence as following:

$$x_k = x_0 + \sum_{j=0}^{k-1} \alpha_j d_j \tag{59}$$

$$\implies (x_k - x_0) = \sum_{j=0}^{k-1} \alpha_j d_j \tag{60}$$

$$\implies d_k^T Q(x_k - x_0) = \sum_{j=0}^{k-1} \alpha_j d_k^T Q d_j = 0 \tag{61}$$

Therefore,

$$\beta_k = \frac{d_k^T Q(x^* - x_0)}{d_k^T Q d_k} \tag{62}$$

$$= \frac{d_k^T Q(x^* - x_0) - d_k^T Q(x_k - x_0)}{d_k^T Q d_k} \tag{63}$$

$$= \frac{d_k^T Q(x^* - x_k)}{d_k^T Q d_k} \tag{64}$$

$$= \frac{d_k^T (Qx^* - Qx_k)}{d_k^T Q d_k} \tag{65}$$

$$= \frac{d_k^T (b - Qx_k)}{d_k^T Q d_k} \qquad \text{(The first order necessary condition suggests } Qx^* = b\text{)}$$

$$= -\frac{d_k^T (Qx_k - b)}{d_k^T Q d_k} \tag{66}$$

$$= -\frac{d_k^T \nabla f(x_k)}{d_k^T Q d_k} \qquad \text{(Assuming } f \text{ is quadratic)}$$

$$= \alpha_k \tag{67}$$

Consequently,

$$x^* = x_0 + \sum_{j=0}^{n-1} \beta_j d_j \tag{68}$$

$$= x_0 + \sum_{j=0}^{n-1} \alpha_j d_j \tag{69}$$

$$= x_n \tag{70}$$

■

7.3.1 Geometric Interpretations of Method of Conjugate Directions

Theorem Let $f \in C^1(\Omega, \mathbb{R})$, where Ω is a convex subset of $\mathbb{R}^n$, then x_0 is a local minimum of f on Ω if and only if

$$\nabla f(x_0) \cdot (y - x_0) \geq 0 \, \forall y \in \Omega$$

Example Now consider the special case in which Ω is an affine hyperplane, that is,

$$\Omega = \{x \in \mathbb{R}^n : cx + b = 0\}$$

where $\dim(\Omega)$ is $n-1$.
Note that for every $y \in \Omega, \nabla f(x_0) \cdot (y - x_0) \geq 0$. For any feasible direction a at point x_0, by definition of hyperplane, $-a$ is a feasible direction as well.
Consequently, $a \cdot \nabla f(x_0) = 0$ for every feasible direction. That is, $\nabla f(x_0) \perp \Omega$. ■

Geometric Interpretation Let $d_0, d_1, \ldots, d_{n-1}$ be a set of non-zero Q-orthogonal vectors in $\mathbb{R}^n$. Let $B_k = Span\{d_0, \ldots, d_{k-1}\}$ for $k = 0, 1, \ldots, n$.
Note:

- $$B_0 = \{0\} \subseteq B_1 = \langle d_0 \rangle \subseteq B_2 = \langle d_0, d_1 \rangle \subseteq \ldots \subseteq B_n = \langle d_0, \ldots, d_{n-1} \rangle = \mathbb{R}^n$$
- $$\dim B_k = k$$
- $$x_0 + B_0 \subseteq x_0 + B_1 \subseteq \ldots$$

Theorem The sequence $\{x_k\}$ generated from $x_0 \in \mathbb{R}^n$ by conjugate directions method has the property that x_k minimizes $f(x) = \frac{1}{2} x^T Q x - b^T x$ on the affine hyperplane $x_0 + B_k$.

Proof. Recall that x_k is the minimizer of $f(x)$ on $x_0 + B_k \iff \nabla f(x_k) \perp x_0 + B_k$
Enough to prove that $\nabla f(x_k) \perp B_k$.
We prove this by induction on k.
Notation: $\nabla f(x_k) = Q x_k - b =: g_k$.
Base case: k = 0 $B_0 = \{0\} \implies g_0 \perp B_0$
Inductive Step: Assume that $g_k \perp B_k$, show $g_{k+1} \perp B_{k+1}$
Since

$$x_{k+1} = x_k + \alpha_k d_k$$

then

$$\underbrace{Q_{k+1} - b}_{g_{k+1}} = \underbrace{Q_{x_k} - b}_{g_k} + \alpha_k Q d_k$$

$$g_{k+1}^T B_k = \langle d_0, \dots, d_{k-1} \rangle \tag{71}$$
$$g_{k+1}^T d_k = (\underbrace{g_k + \alpha_k Q d_k^T d_k}_{g_{k+1}})^T d_k \tag{72}$$
$$= g_k^T d_k + \alpha_k d_k^T Q d_k \tag{73}$$
$$= g_k^T d_k + (-\frac{g_k^T d_k}{d_k^T Q d_k}) d_k^T Q d_k \tag{74}$$
$$= 0 \tag{75}$$

This implies that $g_{k+1} \perp d_k$
For $0 \leq i < k$,

$$g_{k+1}^T \cdot d_i = (g_k + \alpha_k Q d_k)^T d_i \tag{76}$$
$$= \underbrace{g_k^T d_i}_{=0} + \underbrace{\alpha_k d_k^T Q d_i}_{=0} \tag{77}$$
$$= 0 \tag{78}$$

Therefore, $g_{k+1} \perp d_0, d_1, \dots, d_k$
Hence $g_{k+1} \perp \langle d_0, d_1, \dots, d_k \rangle = B_k$ ■

Corollary x_n minimizes $f(x)$ on $x_0 + B_n$ (which is $\mathbb{R}^n$)
i.e. $x_n = x^*$

Corollary $0 \leq q(x_k) = \min_{x \in x_0 + B_k} q(x) \leq q(x_{k-1}) = \min_{x \in x_0 + B_{k-1}} q(x)$

Corollary

$$\begin{cases} \min f(x) \\ x \in x_0 + B_1 \end{cases} \tag{79}$$
$$\implies \begin{cases} \min f(x_0 + td_0) \\ t \in \mathbb{R} \end{cases} \qquad \text{(Since } x_0 + B_1 = \{x_0 + td_0 | t \in \mathbb{R}\}\text{)}$$
$$\implies 0 = \frac{d}{dt}|_{t=t_0} f(x_0 + td_0) = \nabla f(x_0 + t_0 d_0) \cdot d_0 \qquad \text{(where } t_0 \text{ is such that } x_1 = x_0 + t_0 d_0\text{)}$$

■

8 Calculus of Variations

Note: infinite dimensional optimization.

Comparison with finite dimensions

	finite dimensional	∞-dimensional
problem	min $f(x)$	min $F[u]$
constraint	$x \in M$	$u \in \mathcal{A}$
note	set of points in $\mathbb{R}^n$	space of functions

Model model

$$\mathcal{A} = \{u : [0,1] \to \mathbb{R} | u \in C^1 \, s.t. \, u(0) = u(1) = 1\}$$

Note: We call F a "Functional". It maps a function to a real number.

Notation Write $u(\cdot)$ for a function u.

8.1 Example

$F[u(\cdot)] = \frac{1}{2}\int_0^1 \{u(x)^2 + u'(x)^2\}\,dx$.
$\begin{cases} \min F[u(\cdot)] \\ u(\cdot) \in \mathcal{A} \end{cases}$
means: Find $u^*(\cdot) \in \mathcal{A}$ s.t. $F[u^*(\cdot)] \leq F[u(\cdot)]$ for all $u(\cdot) \in \mathcal{A}$.

Plan

1. We derive 1st order necessary conditions for a local min;
2. Find a function $u^*(\cdot)$ satisfying these conditions;
3. Check this candidate $u^*(\cdot)$ is in fact a minimizer.

We reduce this problem to (many) 1-dimensional problems.
Step 1: Derive 1st order necessary conditions for a local min
Fix $v(\cdot) \in C^1$ on $[0,1]$ s.t. $v(0) = 0 = v(1)$.
Suppose $u^*(\cdot) \in \mathcal{A}$ is a minimizer.
Notice that $u^*(\cdot) + sv(\cdot) \in \mathcal{A}\, \forall s \in \mathbb{R}$.
Let $f : \mathbb{R} \to \mathbb{R}$ s.t. $f(s) := F(u^*(\cdot) + sv(\cdot)$.
If $u^*(\cdot)$ minimizes F, then $s = 0$ minimizes f, then $f'(0) = 0$.
Then $f(0) = F[u^*(\cdot)] \leq F[u^*(\cdot) + sv(\cdot)] = f(s)$

$$f'(0) = \frac{d}{ds}|_{s=0} \underbrace{F[u*(\cdot) + sv(\cdot)]}_{f(s)} \tag{80}$$

$$= \frac{d}{ds}|_{s=0} \frac{1}{2}\int_0^1 \{[u^*(x) + sv(x)]^2 + [u^{*'}(x) + sv'(x)]^2\}\,dx \tag{81}$$

$$= \frac{1}{2}\frac{d}{ds}|_{s=0}\int_0^1 \{u^*(x)^2 + u^{*'}(x)^2\}\,dx + \frac{d}{ds}|_{s=0} s\int_0^1 \{u^*(x)v(x) + u^{*'}(x)v'(x)\}\,dx + \frac{d}{ds}|_{s=0}\frac{s^2}{2}\int_0^1 \{v(x)^2 + v'(x)^2\}\,dx \tag{82}$$

$$= \int_0^1 \{u^*(x)v(x) + u^{*'}(x)v'(x)\}\,dx \tag{83}$$

So far, if $u^*(\cdot)$ is a minimizer of F over $\mathcal{A}$, then

$$\int_0^1 \{u^*(x)v(x) + u^{*'}(x)v'(x)\}\,dx = 0 \quad (\heartsuit)$$

for all $v(\cdot) \in C^1$ on $[0,1]$ and $v(0) = 0 = v(1)$. We call this a "primitive form of 1st order condition", and call $v(\cdot)$ the test functions.
Recall Integration by parts:

$$\int_0^1 w(x)v'(x)\,dx = w(x)v(x)|_0^1 - \int_0^1 w'(x)v(x)\,dx$$

$$(\heartsuit) = \int_0^1 u^*(x)v(x)\,dx + \int_0^1 u^{*'}(x)v'(x)\,dx \tag{84}$$

$$= \int_0^1 u^*(x)v(x)\,dx + \underbrace{u^{*'}(x)v(x)|_0^1}_{=0\,(v(0)=v(1)=0)} - \int_0^1 u^{*''}(x)v(x)\,dx \tag{85}$$

$$= \int_0^1 \left(u^*(x) - u^{*''}(x)\right) v(x)\,dx \tag{86}$$

$$= 0 \tag{87}$$

For all test functions $v(\cdot)$.

Lemma: Fundamental Lemma of Calculus of Variations Suppose g is continuous function on interval $[a,b]$. If

$$\int_a^b g(x)v(x)\,dx = 0$$

for all test functions $v(\cdot)$, then
$g(x) \equiv 0$ on $[a,b]$.
Then by Fundamental Lemma of Calculus of Variations, $(\heartsuit) \implies u^*(x) - u^{*''}(x) \equiv 0$, which is the 1st order necessary condition for $u^*(\cdot)$.
Step 2: Find a function $u^*(\cdot)$ satisfying these conditions

$$\begin{cases} u^*(x) = u^{*''}(x) \\ u^*(0) = u^*(1) = 1 \end{cases} \implies u^*(x) = c_1 e^x + c_2 e^{-x} \tag{88}$$

$$\begin{cases} 1 = u^*(0) = c_1 + c_2 \\ 1 = u^*(1) = c_1 e + c_2 \frac{1}{e} \end{cases} \implies c_1 = \frac{1}{e+1}, c_2 = \frac{e}{e+1} \tag{89}$$

$$\implies u^*(x) = \frac{1}{e+1}e^x + \frac{e}{e+1}e^{-x} \tag{90}$$

Step 3: check $u^*(\cdot)$ is in fact a global minimizer.
We derived that

$$F[u^*(\cdot) + sv(\cdot)] = F[u*(\cdot)] + \underbrace{s\int_0^1 \{u^*(x)v(x) + u^{*'}(x)v'(x)\}\,dx}_{=0} + \underbrace{\frac{s^2}{2}\int_0^1 \{v(x)^2 + v'(x)^2\}\,dx}_{\geq 0}$$

$$F[u*(\cdot)] \leq F[u*(\cdot) + sv(\cdot)]$$

for all test functions $v(\cdot)$ and all $s \in real$. In particular, let $s = 1$, then

$$F[u*(\cdot)] \leq F[u^*(x) + v(\cdot)]$$

for all test functions $v(\cdot)$. In particular, let $v(\cdot) = u(\cdot) - u^*(\cdot)$, then

$$F[u*(\cdot)] \leq F[u(\cdot)]$$

for all $u(\cdot) \in \mathcal{A}$.
Note: The space of $v(\cdot)$ is a vector space, but $\mathcal{A}$ is not a vector space (since $u(\cdot) \neq 0$). It is a translate of a vector space.

Lemma: Fundamental Lemma of Calculus of Variations Suppose g is continuous function on interval $[a,b]$. If

$$\int_a^b g(x)v(x)\,dx = 0$$

for all test functions $v(\cdot)$, then
$g(x) \equiv 0$ on $[a,b]$.

Proof. Suppose for contradiction that $g(x) \not\equiv 0$ on $[a,b]$.
WLOG, $g(x_0) > 0$ for some $x_0 \in (a,b)$. This implies that $g > 0$ on $(c,d) \subsetneq (a,b)$.
Let $v(\cdot)$ be a continuous function s.t.

$$v(\cdot) \begin{cases} > 0 & \text{on } (c,d) \\ = 0 & \text{otherwise} \end{cases}$$

Then

$$\int_a^b g(x)v(x)\,dx = \int_c^d \underbrace{g(x)v(x)}_{>0}\,dx > 0$$

which leads to a contradiction. ■

8.2 Classical Problem: the Brachistochrone

Galileo (1638): Find the curve connecting A and B on which a point mass moves without fiction under the influence of gravity in the least time possible.
Johann Bernoulli (1696): Revisit the problem and sent invitations
6 correct solutions sent (1697):
Leibniz, Johann, Jacob, l'Hospital, Von Tschinhaus, Anonymous → Newton (*)
This answer is the beginning of Calculus of Variations

8.3 General class of problems in Calculus of Variations

$$\mathcal{A} = \{u : [a,b] \to \mathbb{R} | u \in C^1, u(a) = A, u(b) = B\}$$

$$F[u(\cdot)] = \int_a^b L(x, u(x), u'(x))\,dx$$

where $L(x,z,p) : [a,b] \times \mathbb{R} \times \mathbb{R} \to \mathbb{R}$

Model example $L(x,z,p) = \frac{z^2+p^2}{2}$, $F[u(\cdot)] = \int_0^1 \frac{u(x)^2+u'(x)^2}{2}\,dx$
Notation:

$$\begin{cases} L_z(x,z,p) = \frac{\partial}{\partial z}L(x,z,p) \\ L_p(x,z,p) = \frac{\partial}{\partial p}L(x,z,p) \end{cases}$$

Definition Given $u(\cdot) \in \mathcal{A}$, suppose $\exists$ function $g(\cdot)$ on $[a,b]$ s.t.

$$\frac{d}{ds}|_{s=0} F[u(\cdot) + sv(\cdot)] = \int_a^b g(x)v(x)\,dx$$

for all test functions $v(\cdot)$, then $g(\cdot)$ is called the variational derivative of F at $u(\cdot)$,
denoted by $\frac{\delta F}{\delta u}(u)(\cdot)$ or $\frac{\delta F}{\delta u}(u)$ or $\frac{\delta F}{\delta u}$.

Analogy **In finite dimensions**:

$$\frac{d}{ds}|_{s=0} f(u+sv) = \nabla f(u)\cdot v \tag{91}$$

$$= \sum_i \nabla f(u)_i v_i \tag{92}$$

for all $v \in \mathbb{R}^n$

In Calculus of Variations (∞ dimensional):

$$\frac{d}{ds}|_{s=0} F[u(\cdot)+sv(\cdot)] = \int_a^b \frac{\delta F}{\delta u}(u)(x)v(x)\,dx \qquad \text{(where possible)}$$

$$\sim \sum_x \frac{\delta F(u)}{\delta u}(x)v(x) \qquad \text{(a kind of an infinite sum)}$$

Model example $L(x,z,p) = \frac{z^2+p^2}{2}$, $F[u(\cdot)] = \int_0^1 \frac{u(x)^2+u'(x)^2}{2}\,dx$

$$\frac{d}{ds}|_{s=0} F[u(\cdot)+sv(\cdot)] = \ldots = \int_0^1 [u(x)-u''(x)]v(x)\,dx$$

for all test functions $v(\cdot)$
Therefore $\frac{\delta F}{\delta u}(u)(x) = u(x)-u''(x)$

Lemma (1st order necessary conditions satisfied by a solution $u^*(\cdot) \in C^1$)

$$\mathcal{A} = \{u : [a,b] \to \mathbb{R} | u \in C^1, u(a) = A, u(b) = B\}$$

If $u^*(\cdot) \in \mathcal{A}$ minimizes F over $\mathcal{A}$, and if $\frac{\delta F}{\delta u}(u^*)(\cdot)$ exists and is continuous, then it must satisfy

$$\frac{\delta F}{\delta u}(u^*)(\cdot) \equiv 0$$

Proof. note: $u^*(\cdot)+sv(\cdot) \in \mathcal{A}$
If $u^*(\cdot)$ is a minimizer of F, then

$$F[u^*(\cdot) \le F[u^*(\cdot)+sv(\cdot)]$$

for all test functions v.
Define $f(s) := F[u^*(\cdot)+sv(\cdot)]$, then $f(0) \le f(s)$ for all $s \in \mathbb{R}$.
Then

$$\int_a^b \frac{\delta F}{\delta u}(u^*)(\cdot)v(x)\,dx = \frac{d}{ds}|_{s=0} F[u^*(\cdot)+sv(\cdot)] \qquad (\tfrac{\partial F}{\partial u}(u^*)(\cdot) \text{ exists})$$

$$= \frac{d}{ds}|_{s=0} f(s) \tag{93}$$

$$= f'(0) = 0 \qquad (0 \text{ is the global minimize of } f)$$

This implies that $\frac{\delta F}{\delta u}(u^*)(\cdot) \equiv 0$. ■

Theorem: Leibniz Integral Rule Let $f(x,t)$ be a function such that both $f(x,t)$ and its partial derivative $\frac{\partial}{\partial x}f(x,t)$ is continuous w.r.t. t and x in some region of the (x,t)-plane, including $a(x) \le t \le b(x), x_0 \le x \le x_1$. Also suppose that the functions $a(x)$ and $b(x)$ are both continuous and both have continuous derivatives for $x_0 \le x \le x_1$. Then, for $x_0 \le x \le x_1$,

$$\frac{d}{dx}\left(\int_{a(x)}^{b(x)} f(x,t)\,dt\right) = f(x,b(x))\cdot\frac{d}{dx}b(x) - f(x,a(x))\cdot\frac{d}{dx}a(x) + \int_{a(x)}^{b(x)}\frac{\partial}{\partial x}f(x,t)\,dt$$

Note that if $a(x)$ and $b(x)$ are constants rather than functions of x, we have a special case of Leibniz's rule:

$$\frac{d}{dx}\left(\int_a^b f(x,t)\,dt\right) = \int_a^b \frac{\partial}{\partial x}f(x,t)\,dt$$

Theorem: Euler-Langrange Equation

$$\mathcal{A} = \{u : [a,b] \to \mathbb{R} | u \in C^1, u(a) = A, u(b) = B\}$$

$$F[u(\cdot)] = \int_a^b L(x, u(x), u'(x))\, dx$$

where $L \in C^2$.
Then if $u(\cdot) \in C^1$, then $\frac{\delta F}{\delta u}(u)(\cdot)$ exists, is continuous, and

$$\frac{\delta F}{\delta u}(u)(x) = -\frac{d}{dx}[L_p(x, u(x), u'(x))] + L_z(x, u(x), u'(x))$$

Then the Euler-Lagrange equation is given by

$$-\frac{d}{dx}[L_p(x, u(x), u'(x))] + L_z(x, u(x), u'(x)) = 0$$

Note: The Euler-Lagrange equation is a second-order PDE whose solutions are the functions for which a given functional is stationary. Because a differentiable functional is stationary at its local maxima and minima, the Euler-Lagrange equation is useful for solving optimization problems in which, given some functional, one seeks the function minimizing or maximizing it. This is analogous to Fermat's Theorem in Calculus, stating that at any point where a differentiable function attains a local extremum its derivative is zero.

Proof. Let v be a test function $(v(a) = v(b) = 0)$

$$\begin{aligned}
\frac{d}{ds}|_{s=0} F[u(\cdot) + sv(\cdot)] &= \frac{d}{ds}|_{s=0} \int_a^b L(x, u(x) + sv(x), u'(x) + sv'(x))\, dx && (94)\\
&= \int_a^b \frac{d}{ds}|_{s=0} L(x, z, p)\, dx && \text{(By Leibniz's rule)}\\
&= \int_a^b L_z(\cdot)v(x) + L_p(\cdot)v'(x)\, dx && (95)\\
&= \int_a^b L_z(\cdot)v(x)\, dx + \int_a^b L_p(\cdot)v'(x)\, dx && (96)\\
&= \int_a^b L_z(\cdot)v(x)\, dx + L_p(\cdot)v(x)|_a^b - \int_a^b \frac{d}{dx} L_p(\cdot)v(x)\, dx && \text{(Integration by parts)}\\
&= \int_a^b [-\frac{d}{dx} L_p(\cdot) + L_z(\cdot)]v(x)\, dx \ \forall \text{ test functions } v(\cdot) && (97)
\end{aligned}$$

By the definition of variational derivative, it follows that

$$\frac{\delta F}{\delta u}(u)(x) = -\frac{d}{dx}[L_p(x, u(x), u'(x))] + L_z(x, u(x), u'(x))$$

Furthermore, since $L(\cdot) \in C^2$, $-\frac{d}{dx} L_p(\cdot)$ and $L_z(\cdot)$ are continuous. Moreover, $u(\cdot)$ and $u'(\cdot)$ are continuous, so is the composite function. Hence the variational derivative is continuous. ■

Model example $L(x, z, p) = \frac{z^2+p^2}{2}$, $F[u(\cdot)] = \int_0^1 \frac{u(x)^2+u'(x)^2}{2}\, dx$
$L_z(x, z, p) = z \implies L_z(x, u(x), u'(x)) = u(x)$
$L_p(x, z, p) = p \implies L_p(x, u(x), u'(x)) = u'(x)$

$$\frac{\delta F}{\delta u}(u(\cdot)) = -\frac{d}{dx}[u'(x)] + u(x) = -u''(x) + u(x)$$

If $u^*(\cdot) \in \mathcal{A}$ is a minimizer, then $-u''(x) + u(x) = 0$

Example 8.1 (min arclength)**.** We will show that the straight line gives the shortest path.

$$\min F[u(\cdot)] = \int_a^b (1+u'(x)^2)^{\frac{1}{2}}\,dx = \text{arclength of } u(\cdot)$$

$$\mathcal{A} = \{u : [a,b] \to \mathbb{R} | u \in C^1, u(a) = A, u(b) = B\}$$

Then $L(x,z,p) = (1+p^2)^{\frac{1}{2}}, L_z = 0$ and $L_p = \frac{p}{(1+p^2)^{\frac{1}{2}}}$
If $u^*(\cdot)$ is a minimizer, then

$$-\frac{d}{dx}\frac{u'(x)}{(1+u'(x))^{\frac{1}{2}}} \equiv 0$$

$\implies \frac{u'(x)}{(1+u'(x))^{\frac{1}{2}}} = const$
$\implies u'(x)^2 = const(1+u'(x)^2)$
Then $u'(x) = \alpha$ for some $\alpha \in \mathbb{R}$.
Then $u(x) = \alpha x + \beta$ for some $\beta \in \mathbb{R}$.

Example 8.2 (Surface Area of Revolution)**.** Suppose $u(\cdot) \in C^1$ on $[a,b]$, the surface area of rotating the curve u connecting a and b can be computed as

$$F[u(\cdot)] = \int_a^b 2\pi u(x)\sqrt{1+u'(x)}\,dx$$

For simplicity, assume $u > 0$. In this example, the space of feasible functions is

$$\mathcal{A} = \{u : [a,b] \to \mathbb{R} : u \in C^1, u(a) = A, u(b) = B, u > 0\}$$

If $u(\cdot)$ solves the minimization problem, it must be the case that

$$\frac{\delta F}{\delta u}(u)(\cdot) \equiv 0 \quad (\dagger)$$

Notice

$$L(x,z,p) = 2\pi z\sqrt{1+p^2}$$
$$L_z(x,z,p) = 2\pi\sqrt{1+p^2}$$
$$L_p(x,z,p) = 2\pi z\frac{p}{\sqrt{1+p^2}}$$

Claim: the family of $u(\cdot) = \beta\cosh(\frac{x-\alpha}{\beta})$ solves the necessary condition †.
Instance 1 When $a = 0, b = 1, A = B = 1$, plugging in the initial condition gives

$$\begin{cases} \beta\cosh\left(\frac{0-\alpha}{\beta}\right) &= 1 \\ \beta\cosh\left(\frac{1-\alpha}{\beta}\right) &= 1 \end{cases} \tag{98}$$

solving above system of equations provides the solution.
Instance 2 When $a = 0, b = 1, A = 1, B = 0$, plugging in these initial conditions gives

$$\begin{cases} \beta\cosh\left(\frac{0-\alpha}{\beta}\right) &= 1 \\ \beta\cosh\left(\frac{1-\alpha}{\beta}\right) &= 0 \end{cases} \tag{99}$$

because $\cosh > 0$, the second equation suggests $\beta = 0$, but in this case the first equation would never hold. Therefore, there is no solution to this calculus of variation.
In face, the surface area is minimized by

$$u(x) = \begin{cases} 1 & \text{if } x = 0 \\ 0 & \text{otherwise} \end{cases} \tag{100}$$

8.4 Euler-Lagrange Equations in $\mathbb{R}^n$

Setup

$$F[u(\cdot)] = \int_a^b L(x, u(x), u'(x))\ dx \tag{101}$$

$$u : [a, b] \to \mathbb{R}^n \tag{102}$$

$$L(x, z, p) : [a, b] \times \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R} \tag{103}$$

$$\mathcal{A} := \left\{u : [a, b] \to \mathbb{R}^n : u \in C^1, u(a) = \mathbf{A}, u(b) = \mathbf{B}\right\} \tag{104}$$

Theorem 8.1 (Euler-Lagrange Equations in Vector Forms)**.**

$$-\frac{d}{dx}\nabla_p L(x, z, p) + \nabla_z L(x, z, p) = \mathbf{0} \in \mathbb{R}^n \quad (\dagger) \tag{105}$$

Example 8.3 (Classical Lagrangian Mechanics)**.**

$$V(x) : \mathbb{R}^n \to \mathbb{R} \text{ potential energy} \tag{106}$$

$$\frac{1}{2}m||v||_2^2 \text{ kinetic energy} \tag{107}$$

$$L(t, x, v) := \frac{1}{2}m||v||_2^2 - V(x) \text{ difference between KE and PE} \tag{108}$$

Consider a path $x(t)$ in $\mathbb{R}^n$, define objective function as

$$F[x(\cdot)] = \int_a^b L(t, x(t), x'(t))\ dt \tag{109}$$

$$= \int_a^b \frac{1}{2}m||\dot{x}(t)||_2^2 - V(x(t))\ dt \tag{110}$$

The Euler-Lagrange equation in vector form implies

$$-\frac{d}{dt}\nabla_{(3)} L(t, x(t), \dot{x}(t)) + \nabla_{(2)} L(t, x(t), \dot{x}(t)) = 0 \tag{111}$$

$$\implies -\frac{d}{dt}m\dot{x}(t) - \nabla V(x(t)) = 0 \tag{112}$$

$$\implies m\ddot{x}(t) = \nabla V(x(t)) \quad (\dagger\dagger) \tag{113}$$

Remark 8.1. (††) is often referred to as *Newtown's second law*: object moves along the path on which the total conversion between kinetic and potential energies is minimized.

Example 8.4 (3-Dimensional Pendulum)**.** Suppose the pendulum is moving on a path such that the total conversion between kinetic and potential energies is minimized, that is

$$\min \int_a^b L(t)\ dt = \int_a^b \frac{1}{2}m(\dot{x}(t)^2 + \dot{y}(t)^2 + \dot{z}(t)^2) - mgz(t)\ dt \tag{114}$$

with the restriction that $||\mathbf{x}(t)|| = \ell$, where ℓ is the radius of the sphere.
The restriction can be embodied by framing the problem using spherical coordinates:

$$x := \ell \cos\varphi \sin\theta \tag{115}$$

$$y := \ell \sin\varphi \sin\theta \tag{116}$$

$$z := -\ell \cos\theta \tag{117}$$

where the path of motion can be characterized using $(\theta(t), \varphi(t))$.
The objective function is therefore

$$L\left(t, \begin{pmatrix}\theta(t)\\ \varphi(t)\end{pmatrix}, \begin{pmatrix}\dot\theta(t)\\ \dot\varphi(t)\end{pmatrix}\right) = \frac{1}{2}m\ell^2(\dot\theta^2 + \dot\varphi^2\sin^2(\theta)) + mg\ell\cos\theta \tag{118}$$

So the Euler-Lagrange equation can be written as

$$-\frac{d}{dt}\nabla_{(3)}L\left(t, \begin{pmatrix}\theta(t)\\ \varphi(t)\end{pmatrix}, \begin{pmatrix}\dot\theta(t)\\ \dot\varphi(t)\end{pmatrix}\right) + \nabla_{(2)}L\left(t, \begin{pmatrix}\theta(t)\\ \varphi(t)\end{pmatrix}, \begin{pmatrix}\dot\theta(t)\\ \dot\varphi(t)\end{pmatrix}\right) = \mathbf{0} \tag{119}$$

8.5 Equality constraints

8.5.1 Isoperimetric constraints

Recall: finite dimensional case

$$f, g : \mathbb{R}^n \to \mathbb{R} \tag{120}$$

$$\begin{cases}\min\limits_{x\in\mathbb{R}^n} & f(x)\\ & g(x) = const\end{cases} \tag{121}$$

Suppose regular point x_* ($\nabla g(x_*) \neq 0$) is a minimizer. Then $\exists\lambda \in \mathbb{R}$ s.t. $\nabla f(x_*) + \lambda\nabla g(x_*) = 0$ (by Lagrange multipliers)

Remark 8.2. x_* minimizes $f + \lambda g$. The Lagrange multipliers convert the original problem to an unconstrained optimization problem $L(x, \lambda) = f(x) + \lambda g(x)$.

Infinite dimensional case

$$F[u(\cdot)] = \int_a^b L^F(x, u(x), u'(x))\,dx \tag{122}$$

$$G[u(\cdot)] = \int_a^b L^G(x, u(x), u'(x))\,dx \tag{123}$$

$$\tag{124}$$

$$\begin{cases}\min\limits_{u(\cdot)\in\mathcal{A}} & F[u(\cdot)]\\ & G[u(\cdot)] = const\end{cases}$$

Suppose regular point $u_*(\cdot)$ ($\frac{\delta G}{\delta u}(u_*) \neq 0$) is a minimizer, then $\exists\lambda \in \mathbb{R}$ s.t.

$$\frac{\delta F}{\delta u}(u_*) + \lambda\frac{\delta G}{\delta u}(u_*) \equiv 0$$

Remark 8.3. u_* minimizes $F + \lambda G$.

Example 8.5.

$$\mathcal{A} := \{u : [-a, a] \to \mathbb{R}, u \in C^1, u(-a) = u(a) = 0\} \tag{125}$$

$$F[u(\cdot)] = \int_a^b u(x)\,dx \tag{126}$$

$$G[u(\cdot)] = \int_a^b \sqrt{1 + u'(x)}\,dx = l > 0 \quad \text{note that } G \text{ is arg length} \tag{127}$$

$$\begin{cases}\min\limits_{u\in\mathcal{A}} & (-F)[u(\cdot)]\\ & G[u(\cdot)] = l\end{cases} \tag{128}$$

Let $u_*(\cdot)$ be a minimizer, then

$$\frac{\delta F}{\delta u} = -\frac{d}{dx}L_p^F + L_z^F$$
$$\frac{\delta G}{\delta u} = -\frac{d}{dx}L_p^G + L_z^G$$

Then Euler-Lagrange equations suggests

$$-\frac{d}{dx}L_p^F + L_z^F + \lambda(-\frac{d}{dx}L_p^G + L_z^G) = 0$$

$$\implies \lambda^2 \frac{u_*'(x)^2}{1+u_*'(x)^2} = (C_1 - x)^2 (\dagger)$$

Claim: Solution $u_*(\cdot)$ to (†) satisfies

$$(x - C_1)^2 + (u_*(x) - C_2)^2 = \lambda^2$$

So that the graph of $u_*(\cdot)$ lies on a circle, and our solution is the semi-circle that has length l.
Check:

$$\frac{d}{dx}\left[2(x - C_1) + 2(u_*(x) - C_2)u_*'(x)\right] = 0 \tag{129}$$

which implies

$$u_*'(x) = -\frac{x - C_1}{u_*(x) - C_2} \tag{130}$$
$$\implies u_*'(x)^2 = \frac{(x - C_1)^2}{(u_*(x) - c_2)^2} \quad (\S) \tag{131}$$

Also,

$$(u_*'(x)^2)(u_*(x) - C_2)^2 = (x - C_1)^2 + (u_*(x) - C_2)^2 = \lambda^2 \tag{132}$$
$$\implies (u_*(x) - C_2)^2 = \frac{\lambda^2}{1 + u_*'(x)^2} \quad (\S\S) \tag{133}$$

Combine (§) and (§§),

$$\frac{\lambda^2}{1 + u_*'(x)^2} u_*'(x)^2 = (x - C_1)^2 \tag{134}$$

It is possible to solve for u:

$$\begin{cases} x = -a, y = 0, (-a - C_1)^2 + (0 - C_2)^2 = \lambda^2 \\ x = +a, y = 0, (+a - C)1)^2 + (0 - C_2)^2 = \lambda^2 \\ \int_{-a}^{a} \sqrt{1 + u'(x)^2}\, dx = l \end{cases}$$

8.5.2 Holonomic constraints