I. Mathematical Preliminaries to Calculus of Variations

In finite-variable optimization (i.e., ordinary optimization that you most likely know as minimization or maximization of functions), we try to find the extremizing (a term that covers both minimizing and maximizing) values of a finite number of scalar variables to get the extremum of a function that is expressed in terms of those variables. That is, we deal with functions of the form $f(x_1, x_2, \cdots, x_n)$ that need to be extremized by finding the extremizing values of $x_1, x_2, \cdots, x_n$. Calculus of variations also deals with minimization and maximization but what we extremize are not functions but functionals.

The concept of a *functional* is crucial to calculus of variations as is a *function* for ordinary calculus of finite number of scalar variables. The difference between a function and a functional is subtle and yet profound. Let us first review the notion of a function in ordinary calculus so that we can understand how the functional is different from it.

In this notes, for presenting mathematical formalisms, we will adopt a format that is different from what is usually followed in applied and engineering mathematics books. That is, instead of introducing a number of seemingly unconnected definitions and concepts first and then finally getting to what we really need, here we will first define or introduce what we actually need and then explain or define the new terms as we encounter them. This takes the suspense out of the notation, definitions, and concepts as they are introduced. New terms are underlined and are immediately explained following their first occurrence. If anything is defined as it is first introduced, it is set in *italics* font.

Because we want to understand the difference between a function and a functional, let us start off with their definitions.

Function

"A rule which assigns a unique real (or complex) number to every $x \in \Omega$ is said to define a real (or complex) *function*."

All is in plain English in the above definition of a function except that we need to say what Ω is. It is called the domain of the function. It is a non-empty open set in $\mathbb{R}^N (\mathbb{C}^N)$.

$\mathbb{R}^N$ (or $\mathbb{C}^N$) is a set of real (or complex) numbers in N dimensions. An element $x \in \mathbb{R}^N$ (or $\mathbb{C}^N$) is denoted by $x = \{x_1, x_2, x_3, \cdots, x_N\}$.

While the notion of a set may be familiar to all those who may read this, the notion of an open set may be new to some.

A set $S \subset \mathbb{C}^N$ is open if every point (or element) of S is the center of an open ball lying entirely in S.

The open ball with center x_0 and radius r in $\mathbb{R}^N$ is the set $\left\{ x \in \mathbb{R}^N \,\middle|\, d_E(x_0, x) < r \right\}$.

$d_E(x, y) = \left\{ \sum_{i=1}^{n} (x_i - y_i)^2 \right\}^{1/2}$ is the Euclidean distance between $x = \{x_1, x_2, x_3, \cdots, x_N\}$ and $y = \{y_1, y_2, y_3, ..., y_N\}$ both belonging to $\mathbb{R}^N$.

This is how we formally define a function. You can notice how many related concepts are needed to define such a simple thing as a function! One should try to relate to these concepts with one's own prior understanding of what a function is. Let us now do this for a functional so that you can see how it is different so that it too becomes as natural and intuitive as a function is to you. A functional is sometimes loosely defined as a function of function(s). But that does not suffice for our purposes because it is subtler than that.

Functional

"A *functional* is a particular case of an operator, in which $R(A) \in \mathbb{R}$ or $\mathbb{C}$." Depending on whether it is real or complex, we define real or complex functionals respectively.

Are you wondering what $R(A)$ is? Read on to find out.

Operator

A correspondence $A(x) = y,\ x \in X,\ y \in Y$ is called an *operator* from one metric space X into another metric space Y, if to each $x \in X$ there corresponds no more than one $y \in Y$.

The set of all those $x \in X$ for which there exists a correspondence $y \in Y$ is called the *domain* of A and is denoted by $D(A)$; the set of all y arising from $x \in X$ is called the *range* of A and is denoted by $R(A)$.

Thus, $R(A) = \{y \in Y;\ y = A(x),\ x \in X\}$

Note also that $R(A)$ is the *image* of $D(A)$ under the operator A.

Now, what is a metric space?

Metric space

A *metric space* is a pair (X, d) consisting of a set X (of points or elements) together with a metric d, which a real valued function $d(x, y)$ defined for any two points $x, y \in X$ and which satisfies the following four properties:

(i) $d(x, y) \geq 0$ ("non-negative")

(ii) $d(x, y) = 0$ if and only if $x = y$ ("zero metric")

(iii) $d(x, y) = d(y, x)$ ("symmetry")

(iv) $d(x, y) \leq d(x, z) + d(z, y)$ where $x, y, z \in X$. ("triangular inequality")

A *metric* is a real valued function $d(x, y),\ \ x, y \in \mathbb{R}^N$ that satisfies the above four properties.

Let us look at some examples of metrics defined in $\mathbb{R}^N$.

1. $d(x, y) = |x - y|$ in $\mathbb{R}$

2. $d(x, y) = \begin{cases} 1 \text{ for } x \neq y \\ 0 \text{ for } x = y \end{cases}$ in $\mathbb{R}$

3. $d(x, y) = \|x - y\| = \sqrt{(x_1 - y_1)^2 + (x_2 - y_2)^2}$ in $\mathbb{R}^2$

4. $d(x, y) = |x_1 - x_2| + |y_1 - y_2|$ also in $\mathbb{R}^2$

We can see that the same $\mathbb{R}$ has two different metrics—the first and second ones in the preceding list. Likewise, the third and fourth are two metrics for $\mathbb{R}^2$. Thus, each real number set in N dimensions can have a number of metrics and hence it can give rise to a number of different metric spaces.

The space X we have used so far is good enough for ordinary calculus. But, in calculus of variations, our unknown is a function. So, we need a new set that is made up of functions. Such a thing is called a *function space*. Let us come to it from something more general than that. We call such a thing a vector space. Let us see what this is. First, note that the vector that we refer to here is not limited to what we usually know in analytical geometry and mechanics as something with a magnitude and a direction.

Vector space

A vector space over a field K is a non-empty set X of elements of any kind (called *vectors*) together with two algebraic operations called vector addition $(\oplus)$ and scalar multiplication $(\odot)$ such that the following 10 properties are true.

1. $x \oplus y \in X$ for all $x, y \in X$. "The set is closed under addition"
2. $x \oplus y = y \oplus x$. "Commutative law for addition"
3. $(x \oplus y) \oplus z = x \oplus (y \oplus z)$ "Associative law for addition"
4. There exists an additive identity θ such that $x \oplus \theta = \theta \oplus x = x$ for all $x \in X$
5. There exists an additive inverse such that $x \oplus x' = x' \oplus x = \theta$
6. For all $\alpha \in K$, and all $x \in X$, $\alpha \odot \mathrm{x} \in \mathrm{X}$ "The set is closed under scalar multiplication".
7. For all $\alpha \in K$, and all $x, y \in X$, $\alpha \odot (\mathrm{x} \oplus \mathrm{y}) = (\alpha \odot x) \oplus (\alpha \odot y)$
8. $(\alpha + \beta) \odot x = (\alpha \odot x) + (\beta \odot x)$ $\alpha, \beta \in K, \quad x \in X$
9. $(\alpha\beta) \odot x = \alpha \odot (\beta \odot x)$
10. There exists a multiplicative identity such that $1 \odot x = x$; and $(0 \odot x \in \theta)$

Pardon the strange symbols that are used for addition and multiplication but that generality is needed so that we don't think in terms of our prior notions of usual multiplications and additions. We use the usual symbols to define a *field*, a term we used above.

A set of elements with two binary operators + and • is called a *field* if it satisfies the following ten properties:

1. $a + b = b + a \qquad a, b \in K$
2. $(a + b) + c = a + (b + c) \qquad a, b, c \in K$
3. $a + 0 = 0 + a = a \qquad a \in K, \quad (\text{"}0 = \text{additive identity"})$
4. $a + (-a) = (-a) + a = 0 \qquad (\text{"additive inverse"})$
5. $a \cdot b = b \cdot a \qquad (\text{"cummutative law"})$
6. $(a \cdot b) \cdot c = a \cdot (b \cdot c)$
7. $a \cdot 1 = 1 \cdot a = a$
8. $a \cdot a^{-1} = a^{-1} \cdot a = 1$ for all $a \in K$ except "0"

9. $a\cdot(b+c)=(a\cdot b)+(a\cdot c)$
10. $(a+b)\cdot c=(a\cdot c)+(b\cdot c)$

Based on the foregoing, we can understand a vector space as a special space of elements (called vectors as already noted) of which the functions that we consider are of just one type.

Next, we consider normed vector spaces, which are simply the counterparts of metric spaces that are defined for normal Euclidean spaces such as $\mathbb{R}^N$.

Normed vector space

A *normed vector space* is a vector space on which a norm is defined.

A *norm* defined on a vector space X is a real-valued function from X to $\mathbb{R}$, i.e., $f:X\to\mathbb{R}$ whose value at $x\in X$ is denoted by $f(x)=\|x\|\in\mathbb{R}$ and has the following properties:

(i) $\|x\|\geq 0$ for all $x\in X$

(ii) $\|x\|=0$ if and only if $x=\theta$

(iii) $\|\alpha x\|=|\alpha|\|x\|$ $\alpha\in K,\ x\in X$

(iv) $\|x+y\|\leq\|x\|+\|y\|$ $x,y\in X$

The above four properties may look trivial. If you think so, try to think of a norm for a certain vector space that satisfies these four properties. It is not as easy as you may think! Later, we will see some examples of norms for function spaces that we are concerned with in this course.

Let us understand more about function spaces.

Function space

A function space is simply a set of functions. We are interested in specific types of function spaces which are vector spaces. In other words, the "vectors" in such vector spaces are functions. Let us consider a few examples to understand what function spaces really are.

1. $C^0[a,b]$ $a,b\in K;$ $\|x\|=\max\limits_{a\leq t\leq b}|x(t)|$

As shown above C^0 is a function space of all continuous functions defined over the interval $[a,b]$. It is a normed vector space with the norm defined as shown. Does this norm satisfy the four properties? Please check for yourself.

2. $C_{\text{int}}{}^0[a,b]$ $a,b\in K;$ $\|x\|=\int_a^b|x(t)|\,dt$

This represents another function space of all continuous functions over an interval. This too is a normed vector space but with a different norm.

3. $C_{\text{int}2}{}^0[a,b]$ $a,b\in K;$ $\|x\|=\sqrt{\int_a^b x^2(t)\,dt}$ has yet another norm and denotes one more function space that is a normed vector space.

4. $C^1[a,b]$ $a,b\in K;$ $\|x\|=\max\limits_{a\leq t\leq b}|x(t)|+\max\limits_{a\leq t\leq b}|\dot{x}(t)|$

Here, $C^1[a,b]$ is a set of all continuous functions that are also differentiable once. Note how the norm is defined in this case. Does this norm satisfy the four properties? Check it out.

Let us now briefly mention some very important classes of function spaces that are widely used in *functional analysis*—a field of mathematical study of functionals. The functionals are of course our main interest here.

Banach space

A complete normed vector space is called a *Banach space*.

A normed vector space X is *complete* if every *Cauchy sequence* from X has a limit in X.

A sequence $\{x_n\}$ in a normed vector space is said to be *Cauchy* (or fundamental) *sequence* if $\|x_n - x_m\| \to 0$ as $n, m \to \infty$

In other words, given $\varepsilon > 0$ there is an integer N such that $\|x_n - x_m\| < \varepsilon$ for all $m, n > N$

$x \in X$ is called a *limit* of a convergent sequence $\{x_n\}$ in a normed vector space if the sequence $\{\|x - x_n\|\}$ converges to zero. In other words, $\lim_{n\to\infty} \|x - x_n\| = 0$.

Verifying if a given normed vector space is a Banach space requires an investigation into the limit of all Cauchy sequences. This needs tools of *real analysis*. We are not going to discuss them here. But let us try to relate to these sequences from a practical viewpoint and why we should worry about them.

In the context of structural optimization, we can imagine the *sequences* (that may or may not be Cauchy sequences) as candidate designs that we obtain in a sequence in iterative numerical optimization. As you may be aware, any numerical optimization technique needs an initial guess which is improved in each iteration. Thus, we get a sequence of "vectors" (functions in our study). Whether such a sequence converges at all or converges to a limit within the space we are concerned with, are important practical questions. The abstract notion of a complete normed vector space helps us in this regard. So, it is useful to know the properties of a function space that we are dealing with. It is one way of knowing if numerical optimization would converge to a limit, which will be our optimal solution.

Hilbert space

A complete inner product space is called a *Hilbert space*.

An *inner product space* (or *pre-Hilbert space*) is a vector space X with an inner product defined on it.

An *inner product* on a vector space X is a mapping $X \times X$ into a scalar field K of X denoted as $\langle x, y \rangle$, $x, y \in X$ and satisfies the following properties:

(i) $\langle x + y, z \rangle = \langle x, z \rangle + \langle y, z \rangle$

(ii) $\langle \alpha x, y \rangle = \alpha \langle x, y \rangle$

(iii) $\langle x, y \rangle = \overline{\langle y, x \rangle}$ The over bar denotes conjugation and is not necessary if x, y are real.

(iv) $\langle x, x \rangle \geq 0$ and

$\langle x, x \rangle = 0$ if and only if $x = \theta$

Note the following relationship between a norm and an inner product.

$$\|x\| = \sqrt{\langle x, x \rangle}$$

Note also the relationship between a metric and an inner product.

$$d(x,y) = \|x-y\| = \sqrt{\langle x-y, x-y \rangle}$$

As an example, for $C^0[a,b]$, the norm and inner product defined as follows.

$$\|x\| = \sqrt{\int_a^b x^2(t)\,dt} = \sqrt{\langle x,x \rangle}$$

$$\langle x,y \rangle = \int_a^b x(t)y(t)\,dt$$

Thus, inner product spaces are normed vector spaces. Likewise, Hilbert spaces are Banach spaces.

Normed vector spaces give us the tools for algebraic operations to be performed on vector spaces because we have the notion of how close things ("vectors") are to each other by way of norm. Inner product spaces enable us to do more; they allow us to study the geometric aspects. As an example, consider that orthogonality (or perpendicularity) or lack of it is easily noticeable from the inner product.

For $x, y \in X$, if $\langle x,y \rangle = 0$, then x is said to be orthogonal to y

Banach and Hilbert spaces are classes of useful function spaces (again remember that a function space is only one type of the more general concept of a vector space). There are also some specific function spaces that we should be familiar with as they are the spaces to which the design spaces that we consider in structural optimization actually belong.

Lebesgue space

A *Lebesgue space* defined next is a Banach space.

$$L^q(\Omega) = \left\{ v : v \text{ is defined on } \Omega \text{ and } \|v\|_{L^q(\Omega)} < \infty \right\} \text{ where } \|v\|_{L^q(\Omega)} = \left(\int_\Omega \left| v(x)^q \right| dx \right)^{1/q} \qquad 1 \le q \le \infty$$

The case of $q = 2$ gives $L^2(\Omega)$ consisting of all square-integrable functions. The integration of square of a function is important for us as it often gives the energy of some kind. Think of kinetic energy which is a scalar multiple of the square of the velocity. On many occasions, we also have other energies (usually potential energies or strain energies) that are squares of derivatives of functions. This gives us a number of energy spaces. The Sobolev space gives us exactly that.

Sobolev space

$$W^{r,q}(\Omega) = \left\{ v \in L^1(\Omega) : \|v\|_{W^{r,q}(\Omega)} < \infty \right\}, \qquad 1 \le q \le \infty$$

where

$$\|v\|_{W^{r,q}(\Omega)} = \left(\sum_{|\alpha| \le r} \|D^\alpha v\|^q_{L^q(\Omega)} \right)^{1/q} \text{ is the \textit{Sobolev norm}}$$

$$L^1(\Omega) = \left\{ v : v \in L^1(K) \text{ for any compact } K \text{ inside } \Omega \right\}$$

D^α used above denoted the derivative of order α. Sobolev space is a Banach space.

Note: We have used the qualifying word "compact" for K above. A closed and bounded set is called a compact set. We will spare us from the definitions of closedness and boundedness of a set because we have already deviated from our main objective of knowing what a functional is. Let us return to functionals now.

We have defined a functional as a particular case of an operator whose range is a real (or complex) number set. Let us also consider another definition which says the same thing but in a different way as we have talked much about vector spaces and fields.

Functional—another definition

A *functional* J is a transformation from a vector space to its coefficient field $J : X \to K$.

Let us now look at certain types of functionals that are of main interest to us.

A *linear functional* is one for which

$J(x+y) = J(x) + J(y)$ for all $x, y \in X$ and $J(\alpha x) = \alpha J(x)$ for all $\alpha \in K,\ x \in X$ hold good. Some people write the above two linearity properties as a single property as follows.

$$J(\alpha x + \beta y) = \alpha J(x) + \beta J(y) \quad \text{for all } x, y \in X;\ \alpha, \beta \in K$$

A definite integral is a linear functional. We will deal with a lot of definite integrals in calculus of variations as well as variational methods and structural optimization.

A *bounded functional* is one when there exists a real number c such that $|J(x)| \le c\|x\|$ where $|\cdot|$ is the norm in K; $\|\cdot\|$ is the norm in X.

Continuous functional

Now, we have discussed in which function spaces our functions reside. In calculus of variations, our unknowns are functions. Our objective is a functional. Just as in ordinary finite-variable optimization, in calculus of variations too we need to take derivatives of functionals. What is the equivalent of a derivative for a functional? Before we define such a thing, we need to understand the concept of continuity for a functional. We do that next.

A functional J is said to be continuous at x in D (an open set in a given normed vector space X) if J has the limit $J(x)$ at x. Or symbolically, $\lim_{y \to x \in X} J(y) = J(x)$.

J is said to be *continuous* on D if J is continuous at each vector in D

J has the limit L at x if for every positive number ε there is a ball $B_r(x)$ (with radius r) contained in D such that $|L - J(y)| < \varepsilon$ for all $y \in B_r(x)$. Or symbolically, $\lim_{y \to x \in X} J(y) = L$.

II. First variation of functionals

The derivative of a function being zero is a necessary condition for the extremum of that function in ordinary calculus. Let us now consider the equivalent of a derivative for functionals because it plays the same crucial role in calculus of variations as does the derivative of the ordinary calculus in minimization of functions. Let us begin with a simple but a very important concept called a Gâteaux variation.

Gâteaux variation

The functional $\delta J(x)$ is called the Gâteaux variation of J at x when the limit that is defined as follows exists.

$$\delta J(x;h) = \lim_{\varepsilon \to 0} \frac{J(x+\varepsilon h) - J(x)}{\varepsilon} \quad \text{where } h \text{ is any vector in a vector space, } X .$$

Let us look at the meaning of h and ε geometrically. Note that $x, h \in X$. Now, since x is the unknown function to be found so as to minimize (or maximize) a functional, we want to see what happens to the functional $J(x)$ when we perturb this function slightly. For this, we take another function h and multiply it by a small number ε. We add εh to x and look at the value of $J(x+\varepsilon h)$. That is, we look at the perturbed value of the functional due to perturbation εh. Symbolically, this is the shaded area shown in Fig. 1 where the function x is indicated by a thick solid line, h by a thin solid line, and $x+\varepsilon h$ by a thick dashed line. Next, we think of the situation of ε tending to zero. As $\varepsilon \to 0$, we consider the limit of the shaded area divided by ε. If this limit exists, such a limit is called the Gâteaux variation of $J(x)$ at x for an arbitrary but fixed vector h. Note that, we denote it as $\delta J(x;h)$ by including h in defining Gâteaux variation.

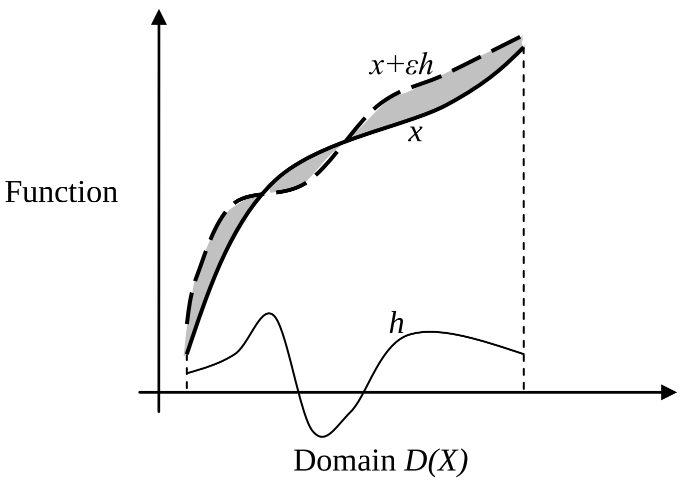

Figure 1. Pictorial depiction of variation εh of a function x

Although the most important developments in calculus of variations happened in 17th and 18th centuries, this formalistic concept of variation was put forth by a French mathematician Gâteaux around the time of the First World War. So, one can say that intuitive and creative thinking leads to new developments and rigorous thinking makes them mathematically sound and completely unambiguous. To reinforce our understanding of the Gâteaux variation, let us relate it to the concept of a directional derivative in multi-variable calculus.

A directional derivative of the function $f(x_1, x_2, ..., x_n)$ denoted in a compact form as $\nabla_{\bar{h}} f(\bar{x})$ in the direction of a given vector $\bar{h}$ is given by

$$\lim_{\varepsilon \to 0} \frac{f(\bar{x}+\varepsilon\bar{h}) - f(\bar{x})}{\varepsilon}.$$

Here the "vector" is the usual notion that you know and not the extended notion of a "vector" in a vector space. We are using the over-bar to indicate that the denoted quantity consists of several elements in an array as in a column (or row) vector. You know how to take the derivative of a function $f(\bar{x})$ with respect to any of its variables, say $x_i, 1 \le i \le n$. It is simply a partial derivative of $f(\bar{x})$ with respect to x_i. You also know that this partial derivative indicates the rate of change of $f(\bar{x})$ in the direction of x_i. What if you want to know the rate of change of $f(\bar{x})$ in some arbitrary direction denoted by $\bar{h}$? This is exactly what a directional derivative gives. Indeed, $\nabla_{\bar{h}} f(\bar{x}) = \nabla_{\bar{h}} f(\bar{x}) \cdot \bar{h} = \nabla_{\bar{h}} f(\bar{x})^T \bar{h}$. That is, the component of the gradient in the direction of $\bar{h}$.

Now, relate the concept of the directional derivative to Gâteaux variation because we want to know how the value of the functional changes in a "direction" of another element h in the vector space. Thus, the Gateaux variation extends the concept of the directional derivative of finite multi-variable calculus to infinite dimensional vector spaces, i.e., calculus of functionals.

Gâteaux differentiability

If Gateaux variation exists for all $h \in X$ then J is said to be Gateaux differentiable.

Operationally useful definition of Gâteaux variation

Gateaux variation can be thought of as the following ordinary derivative evaluated at $\varepsilon = 0$.

$$\delta J(x;h) = \frac{d}{d\varepsilon} J(x+\varepsilon h)\Big|_{\varepsilon=0}$$

This helps calculate the Gâteaux variation easily by taking an ordinary derivative instead of evaluating the limit as in the earlier formal definition. Note that this definition follows from the earlier definition and the concept of how an ordinary derivative is defined in ordinary calculus if we think of the functional as a simple function of ε.

Gâteaux variation and the necessary condition for minimization of a functional

Gâteaux variation provides a necessary condition for a minimum of a functional.

Consider $J(x)$ where $J(x)$, $x \in D$, is an open subset of a normed vector space X, and $x^* \in D$ and any fixed vector $h \in X$.

If x^* is a minimum, then

$$J\left(x^*+\varepsilon h\right)-J\left(x^*\right)\geq 0$$

must hold for all sufficiently small ε

Now,
for $\varepsilon \geq 0$

$$\frac{J\left(x^*+\varepsilon h\right)-J\left(x^*\right)}{\varepsilon}\geq 0$$

and for $\varepsilon \leq 0$

$$\frac{J\left(x^*+\varepsilon h\right)-J\left(x^*\right)}{\varepsilon}\leq 0$$

If we let $\varepsilon \to 0$,

$$\left.\begin{array}{l}\lim\limits_{\substack{\varepsilon\to 0\\ \varepsilon>0}}\dfrac{J\left(x^*+\varepsilon h\right)-J\left(x^*\right)}{\varepsilon}\geq 0\\ \text{and}\quad \lim\limits_{\substack{\varepsilon\to 0\\ \varepsilon<0}}\dfrac{J\left(x^*+\varepsilon h\right)-J\left(x^*\right)}{\varepsilon}\leq 0\end{array}\right\}\underbrace{\lim_{\varepsilon\to 0}\frac{J\left(x^*+\varepsilon h\right)-J\left(x^*\right)}{\varepsilon}}_{\substack{\text{Gâteaux variation}\\ \text{ensures the existence of this limit}}}=\delta J(x;h)=0$$

This simple derivation proves that the Gâteaux variation being zero is the necessary condition for the minimum of a functional. Likewise we can show (by simply reversing the inequality signs in the above derivation) that the same necessary condition applies to maximum of a functional.

Now, we can state this as a theorem since it is a very important result.

Theorem: necessary condition for a minimum of a functional

$$\delta J\left(x^*;h\right)=0 \quad \text{for all } h\in X$$

Based on the foregoing, we note that the Gâteaux variation is very useful in the minimization of a functional but the existence of Gateaux variation is a weak requirement on a functional since this variation does not use a norm in X. Thus, it is not directly related to the continuity of a functional. For this purpose, another differential called Fréchet differential has been put forth.

Frechet differential

$$\lim_{\|h\|\to 0}\frac{J\left(x+h\right)-J\left(x\right)-dJ\left(x;h\right)}{\|h\|}=0$$

If the above condition holds and $dJ(x;h)$ is a linear, continuous functional of h, then J is said to be Fréchet differentiable at x with "increment" h.

$dJ(x;h)$ is called the Fréchet differential.

If J is differentiable at each $x \in D$ we say that J is Fréchet differentiable in D.

Some properties of Fréchet differential

i) $J(x+h) = J(x) + dJ(x;h) + E(x;h)\|h\|$ for any small non-zero $h \in X$ has a limit zero at the zero vector in X. That is,

$$\lim_{h \to \theta} E(x;h) = 0.$$

Based on this, sometimes the Fréchet differential is also defined as follows.

$$\lim_{h \to \theta} \frac{J(x+h) - J(x) - dJ(x;h)}{\|h\|} = 0.$$

ii) $dJ(x; a_1 h_1 + a_2 h_2) = a_1 dJ(x;h_1) + a_2 dJ(x;h_2)$ must hold for any numbers $a_1, a_2 \in K$ and any $h_1, h_2 \in X$.
This is simply the linearity requirement on the Fréchet differential.

iii) $dJ(x;h) \le \text{c} \; \|h\|$ for all $h \in X$, where c is a constant.
This is the continuity requirement on the Fréchet differential.

iv) $|dJ(x;h)| = \underbrace{J'(x)}_{\substack{\text{Frechet}\\ \text{derivative}}} h$

This is to say that the Fréchet differential is a linear functional of h. Note that it also introduces a new definition: Fréchet derivative, which is simply the coefficient of h in the Fréchet differential.

Relationship between Gâteaux variation and Fréchet differential

If a functional J is Fréchet differentiable at x then the Gateaux variation of J at x exists and is equal to the Fréchet differential. That is,

$$\delta J(x;h) = dJ(x;h) \quad \text{for all} \quad h \in X$$

<u>Here is why:</u>

Due to the linearity property of $dJ(x;h)$, we can write

$$dJ(x;\varepsilon h) = \varepsilon dJ(x;h)$$

By substituting the above result into property (i) of the Fréchet differential noted earlier, we get

$$J(x+\varepsilon h) - J(x) - \varepsilon dJ(x;h) = E(x,\varepsilon h)\|h\|\,|\varepsilon| \qquad \text{for any } h \in X$$

A small rearrangement of terms yields

$$\frac{J(x+\varepsilon h) - J(x)}{\varepsilon} = dJ(x;h) + E(x,\varepsilon h)\|h\|\frac{|\varepsilon|}{\varepsilon}$$

When limit $\varepsilon \to 0$ is taken, the above equation gives what we need to prove:

$$\lim_{\varepsilon\to 0}\frac{J(x+\varepsilon h) - J(x)}{\varepsilon} = \delta J(x;h) = dJ(x;h) \quad \text{because} \quad \lim_{\varepsilon\to 0} E(x,\varepsilon h)\|h\|\frac{|\varepsilon|}{\varepsilon} = 0$$

Note that the latter part of property (i) is once again used in the preceding equation.

Operations using Gateaux variation

Consider a simple general functional of the form shown below.

$$J(y) = \int_{x_1}^{x_2} F(x,\ y(x),\ y'(x))\ dx$$

where $y'(x) = \dfrac{dy}{dx}$

Note our sudden change of using x. It is no longer a member (element, vector) of a normed vector space X. It is now an independent variable and defines the domain of $y(x)$, which is a member of a normed vector space. Now, $y(x)$ is the unknown function using which the functional is defined. We need to have our wits about us to see which symbol is used in what way!

If we want to calculate the Gâteaux variation of the above functional, instead of using the formal definition that needs an evaluation of the limit we should use the alternate operationally useful definition—taking the ordinary derivative of $J(y+\varepsilon h)$ with respect to ε and evaluating at $\varepsilon = 0$. In fact, there is an easier route that is almost like a thumb-rule. Let us find that by using the derivative approach for the above simple functional.

$$J(y+\varepsilon h) = \int_{x_1}^{x_2} F(x,\ y(x)+\varepsilon h(x), y'(x) + \varepsilon h'(x))\ dx$$

Recalling that $\delta J(x;h) = \dfrac{d}{d\varepsilon} J(x+\varepsilon h)\Big|_{\varepsilon=0}$, we can write

$$\frac{d}{d\varepsilon}J\left(x+\varepsilon h\right)=\frac{d}{d\varepsilon}\left\{\int_{x_1}^{x_2}F\left(x,\ y+\varepsilon h, y'+\varepsilon h'\right)\ dx\right\}$$
$$=\int_{x_1}^{x_2}\frac{d}{d\varepsilon}\left\{F\left(x,\ y+\varepsilon h, y'+\varepsilon h'\right)\right\}\ dx$$

Please note that the order of differentiation and integration have been switched above. It is a legitimate operation. By using chain-rule of differentiation for the integrand of the above functional, we can further simplify it to obtain

$$\delta J\left(x;h\right)=\int_{x_1}^{x_2}\left(\frac{\partial F}{\partial\left(y+\varepsilon h\right)}h+\frac{\partial F}{\partial\left(y'+\varepsilon h'\right)}h'\right)\Bigg|_{\varepsilon=0}=\int_{x_1}^{x_2}\left(\frac{\partial F}{\partial y}h+\frac{\partial F}{\partial y'}h'\right)dx\,.$$

What we have obtained above is a general result in that for any functional, be it of the form $J(x,y,y',y'',y''',\cdots)$, we can write the variation as follows.

$$\delta J\left(x;h\right)=\int_{x_1}^{x_2}F(x,y,y',y'',y''',\cdots)dx=\int_{x_1}^{x_2}\left(\frac{\partial F}{\partial y}h+\frac{\partial F}{\partial y'}h'+\frac{\partial F}{\partial y''}h''+\frac{\partial F}{\partial y'''}h'''+\cdots\right)dx\,.$$

Note that in taking partial derivatives with respect to y and its derivatives we treat them as independent. It is a thumb-rule that enables us to write the variation rather easily by inspection and using rules of partial differentiation of ordinary calculus.

We have now laid the necessary mathematical foundation for deriving the Euler-Lagrange equations that are the necessary conditions for the extremum of a function. Note that the Gâteaux variation still has an arbitrary function h. When we get rid of this, we get the Euler-Lagrange equations. For that we need to talk about fundamental lemmas of calculus of variations.

III. Fundamental lemmas of calculus of variations

We are now familiar with the notions of a functional, vector spaces (of which function spaces are one type), Gâteaux variation and Fréchet differential. We also know operationally useful definition of Gâteaux variation of a functional. We did all this because we want to derive the necessary conditions for a minimum of the given functional. But then, Gâteaux variation depends on an arbitrary function h. In contrast, the gradient (i.e., the derivative) of an ordinary function does not have such an arbitrary entity. Of course, we noted that h exists in the definition of Gâteaux variation just as a direction is there in the definition of a directional derivative of an ordinary function. In any case, h is there and we have to deal with it. At this point, h is there in between us and the necessary conditions for a minimum of a functional. This is where the fundamental lemma of calculus of variations helps us to get h out of the picture. So, let us look at it.

Lemma 1

If $F(x)$ is continuous in $[a,b]$ and if $\int_a^b F(x)h(x)\,dx = 0$ for every function $h(x) \in c^0(a,b)$ such that $h(a) = h(b) = 0$, then $F(x) = 0$ for all $x \in [a,b]$.

It is a simple but profound statement. It is simple in that one can easily see why this is true. It is profound because many results of calculus of variations rest on this. It is interesting to note that its proof was attempted in 1854 by Stegmann before Du Bois-Raymond rigorously proved it in 1879. So, we can perhaps assume that Euler, Lagrange and others who dealt with necessary and sufficient conditions for a minimum of a functional tacitly assumed that it is true. For the sake of completeness, let us look at a proof of this lemma. It will be proved by contradiction—a legitimate method of proving things. Incidentally, *proof by contradiction* is simply a process of verifying what you know as truth!

Proof of lemma 1 by contradiction

Let us say that $F(x)$ is not zero over its entire domain. Let us assume that it is positive for some interval $[x_1, x_2]$ contained within $[a,b]$. Let $h(x) = (x - x_1)(x_2 - x)$ for $x \in [x_1, x_2]$ and zero outside of $[x_1, x_2]$. Note that $(x - x_1)(x_2 - x)$ is positive for $x \in [x_1, x_2]$. Now, consider:

$$\int_a^b F(x)h(x)\,dx = \int_a^{x_1} F(x)h(x)\,dx + \int_{x_1}^{x_2} F(x)h(x)\,dx + \int_{x_2}^{b} F(x)h(x)\,dx$$

$$= 0 + \int_{x_1}^{x_2} F(x)h(x)dx + 0$$

$$= \int_{x_1}^{x_2} F(x)(x-x_1)(x_2-x)\,dx > 0$$

Thus, we get a contradiction to what is given in the lemma. So, we can conclude that $F(x)$ cannot be non-zero anywhere in the domain $[a,b]$. This proves the lemma.

Lemma 2

If $F(x)$ is continuous in $[a,b]$ and if $\int_a^b F(x)h'(x)\,dx = 0$ for every $h(x) \in c^1(a,b)$ such that $h(a) = h(b) = 0$, then $F(x)$ = constant for all $x \in [a,b]$.

To prove this, let c be defined as in $\int_a^b (F(x)-c)dx = 0$ and let $h(x) = \int_a^x (F(\xi)-c)d\xi$ so that $h(x)$ satisfies the conditions laid out in the statement of the lemma. Now, consider:

$\int_a^b (F(x)-c)\,h'(x)dx = \int_a^b F(x)h'(x)dx - c\{h(b)-h(a)\} = 0$ (Why is this true? The reason lies in the statement of the lemma.)

and

$\int_a^b (F(x)-c)\,h'(x)dx = \int_a^b (F(x)-c)^2\,dx$ (Why is this true? The reason lies in our assume $h(x)$.)

Therefore, $\int_a^b (F(x)-c)\,h'(x)dx = \int_a^b (F(x)-c)^2\,dx = 0 \Rightarrow F(x)-c = 0 \Rightarrow F(x) = c$ for all $x \in [a,b]$. This proved this second lemma.

In calculus of variations, two more lemmas are also stated.

Lemma 3

If $F(x)$ is continuous in $[a,b]$ and if $\int_a^b F(x)h''(x)dx = 0$ for every $h(x) \in c^2(a,b)$ such that $h(a) = h(b) = 0$ and $h'(a) = h'(b) = 0$, then $F(x) = c_0 + c_1 x$ for all $x \in [a,b]$ where c_0 and c_1 are constants.

Lemma 4

If $F_1(x)$ and $F_2(x)$ are continuous in $[a,b]$ and if $\int_a^b \left[F_1(x)h(x) + F_2(x)h'(x)\right]dx = 0$ for every $h(x) \in c^1(a,b)$ such that $h(a) = h(b) = 0$, then $F_2(x)$ is differentiable and $F_2'(x) = F_1(x)$ for all $x \in [a,b]$.

Lemmas 3 and 4 can also be proved by contradiction in the same way as the first two by assuming certain functions for $h(x)$. It is also interesting that lemmas 2-4 can also be derived from lemma 1 using the simple rule of integration by parts. In fact, as we will see later in the course, the rule of integration by parts is an essential tool of calculus of variations. We must also recall that Green's theorem and divergence theorem are essentially integration by parts in higher dimensions.

IV. Variational Derivative

We have studied Gâteaux variation and Fréchet differential and the relationship between them. There is one more subtle variant of this, which is called variational derivative. It is useful in some applications and in proving some theorems. More importantly, it tells us an alternative way of looking at the concept of variation based purely on the techniques of ordinary calculus. In fact, it can be interpreted as the "partial derivative" equivalent for calculus of variations. As the history goes, Euler had apparently derived his eponymous necessary condition using this concept.

Let us begin with the notation. The variational derivative of a functional $J = \int_{x_0}^{x_f} F(x, y, y')dx$ is denoted as $\frac{\delta J}{\delta y}$ and is given by

$$\frac{\delta J}{\delta y} = F_y - \frac{d}{dx}(F_{y'}) \tag{1}$$

You can immediately see that it is nothing but the E-L expression that should be zero. When J has a more general form, the expression for $\frac{\delta J}{\delta y}$ will be the corresponding expression in the E-L equation that we equate to zero. Let us see what rationale underlies this definition.

Because we want to use only the techniques of ordinary calculus, let us "discretize" $y(x)$ and consider finitely many discrete points $x_k \left(k = 1, 2, ..., N\right)$ within the interval $\left(x_0, x_f\right)$. See Fig. 1. As can be seen in this figure, by way of discretization, we are approximating the continuous curve of $y(x)$ by a polygon.

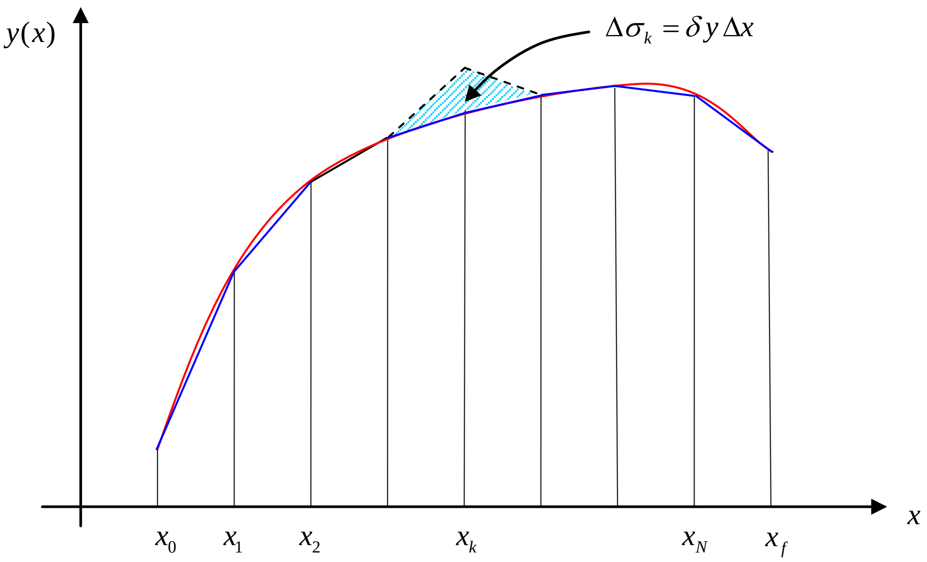

Figure 1. Discretization of a continuous curve $y(x)$ by a polygon. All subdivisions on the x-axis are equal to Δx. A local perturbation at x_k is considered and its effect is shown with the dashed lines.

Now, the functional can be approximated as follows.

$$\sum_{k=1}^{N} J \approx J_N = \sum_{k=1}^{N} F\left(x_k, y_k, \frac{(y_{k+1}-y_k)}{(x_{k+1}-x_k)} \right)(x_{k+1}-x_k) = \sum_{k=1}^{N} F\left(x_k, y_k, \frac{(y_{k+1}-y_k)}{\Delta x} \right)\Delta x \quad (2)$$

where in the last step we have assumed that all subdivisions along the x-axis are equal to Δx. Our variables to minimize J_N are now $\{y_1, y_2, \cdots, y_N\}$. Consider the partial derivative of J_N with respect to y_k.

$$\frac{\partial J_N}{\partial y_k} = F_y(x_k, y_k, \frac{(y_{k+1}-y_k)}{\Delta x})\Delta x + F_{y'}(x_{k-1}, y_{k-1}, \frac{(y_k - y_{k-1})}{\Delta x}) - F_{y'}(x_k, y_k, \frac{(y_{k+1}-y_k)}{\Delta x}) \quad (3)$$

Here, we have only used the chain rule of differentiation. As $\Delta x \to 0$, the RHS of Eq. (3) goes to zero. Now, divide the LHS and RHS of Eq. (3) by Δx to get

$$\frac{\partial J_N}{\partial y_k \Delta x} = F_y(x_k, y_k, \frac{(y_{k+1}-y_k)}{\Delta x}) + \frac{F_{y'}(x_{k-1}, y_{k-1}, \frac{(y_k - y_{k-1})}{\Delta x}) - F_{y'}(x_k, y_k, \frac{(y_{k+1}-y_k)}{\Delta x})}{\Delta x} \quad (4)$$

When $\Delta x \to 0$, $\partial y_k \Delta x$, which can be interpreted as the shaded area in Fig. 1, also tends to zero. In fact, we then denote $\partial y_k \Delta x$ as $\Delta \sigma_k$ or, in general, simply as $\delta y \Delta x$ evaluated at $x = x_k$. Furthermore, as $\Delta x \to 0$, $J_N \to J$. We take the limit of Eq. (4) as $\Delta x \to 0$.

$$\lim_{\Delta x \to 0} \frac{\partial J_N}{\partial y_k \Delta x} = \frac{\delta J}{\delta y} = F_y - \frac{d}{dx}\left(F_{y'}\right) \quad (5)$$

Notice how we defined the variational derivative in Eq. (5). We can think of $\frac{\delta J}{\delta y}$ as the limiting case of $\frac{J(y+h) - J(y)}{\Delta \sigma}$ where h is the perturbation (i.e., variation) of y at some $\hat{x}$ and $\Delta \sigma$ is the extra area under $y(x)$ due to that perturbation. Therefore, we write

$$\Delta J = J(y+h) - J(y) = \left\{ \left.\frac{\delta J}{\delta y}\right|_{x=\hat{x}} + \varepsilon \right\} \Delta \sigma \quad (6)$$

where ε is a small discretization error. When the discretization error is insignificantly small, we can write

$$\Delta J \approx \left.\frac{\delta J}{\delta y}\right|_{x=\hat{x}} \Delta \sigma \quad (7)$$

Thus, the variational derivative helps us get the first order change in the value of the functional for a local perturbation of $y(x)$ at $x = \hat{x}$. Think of Taylor series of expansion of a function of many variables and try to relate this concept of first order change in the value of the function.