When linear algebra meets calculus

We have seen that we need to contend with differential equations. Writing conservation laws with differential equations imposes a requirement for the behavior of the functions (fields such as $p, T, \vec{v}, \rho$) that we are solving for.

In this section, we will:

(-) discuss continuity of functions and how it relates to their differentiability

(-) use their continuous nature to develop efficient methods of solution to differential equations.

A. Continuous functions:

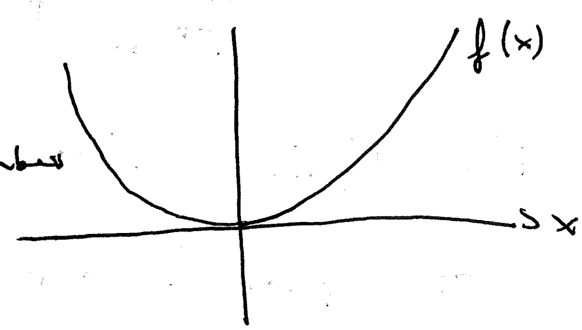
A continuous fct is one you can draw the graph of without needing to lift your pen from the page... not very technical

Mathematically, one uses limits to define continuity

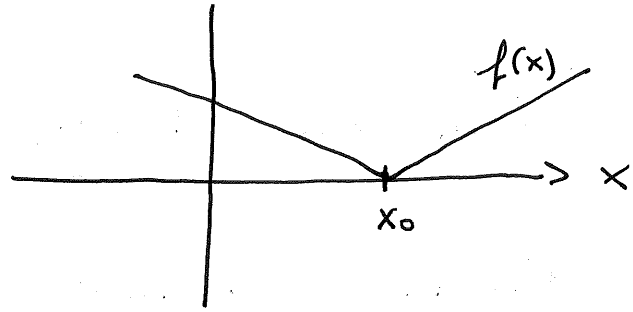
if $\lim_{x \to x_0} f(x) = f(x_0)$ the function $f(x)$ is continuous at x_0!

Examples: $f(x) = x^2$

is continuous over Real numbers



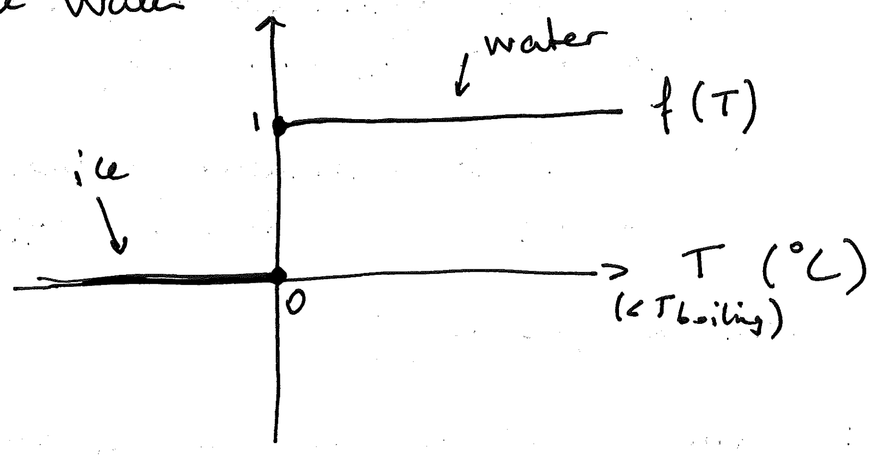
$$f(x) = |x - x_0|$$



is also continuous over $\mathbb{R}$

Imagine now $H(T)$, the enthalpy of a pure substance (water) as function of temperature T, specifically we will look into how melt fraction (= mass fraction of water in the liquid state) evolves around the phase change at $0°C$ ($p = p_{atm}$)

For pure water



If we start from negative T, $T_0^- < 0$

$$\lim_{T_0^- \to 0} f(T) = 0$$

If we start from $T_0^+ > 0$

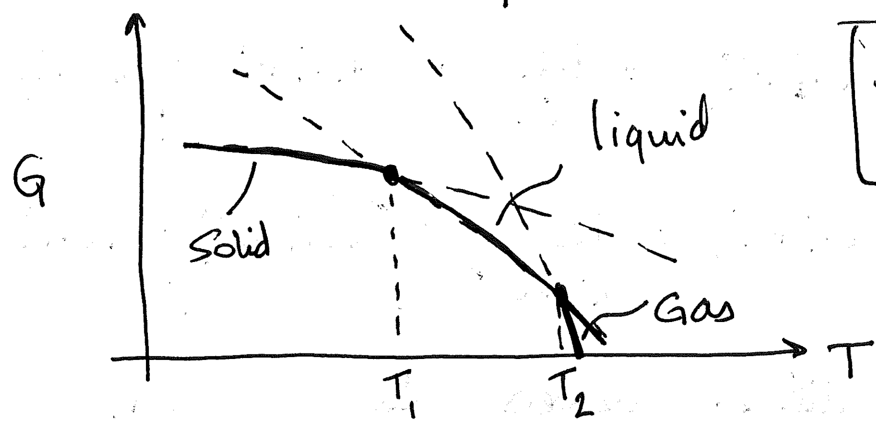
$$\lim_{T_0^+ \to 0} f(T) = 1$$

$\neq$

The limit $T \to 0$ $\lim_{T \to 0} f(T)$ is not unique

$\Rightarrow$ $f(T)$ is not continuous at $T = 0$.

However, Gibbs free energy $G(p,T,N)$ vs T is continuous



$\boxed{\text{1st order phase change}}$

T_1 = T of fusion
T_2 = T of vaporization

$$dG = Vdp - SdT + \mu dN$$

Using the fact that G has a total derivative dG (see Fundamental Theorem of Calculus)

$$\left(\frac{\partial G}{\partial p}\right)_{T,N} = V \; ; \; \boxed{\left(\frac{\partial G}{\partial T}\right)_{p,N} = -S} \; ; \; \left(\frac{\partial G}{\partial N}\right)_{p,T} = \mu$$

For first order phase change we can see that

at fixed (p,N): if we consider $T_0^- \rightarrow T_0^- < T_1$
$T_0^+ \rightarrow T_0^+ > T_1$

$$\lim_{T_0^- \to T_1} S \neq \lim_{T_0^+ \to T_1} S$$

$\Rightarrow$ Gibbs free energy G is continuous at T_1

<u>BUT</u> entropy S is not!

say $h^+ > 0$ (so that $\overset{T > T_1}{T = T_1 + h^+}$) @ fixed p, N

$$\lim_{h^+ \to 0} S(T_1 + h^+) = \lim_{h^+ \to 0} - \left[\frac{G(T_1 + h^+) - G(T_1)}{h^+} \right]_{p,N}$$

$\underset{T = T_1 + h^-}{T < T_1}$: $$\lim_{h^- \to 0} S(T_1 + h^-) = \lim_{h^- \to 0} - \left[\frac{G(T_1 + h^-) - G(T_1)}{h^-} \right]_{p,N}$$

provide different answers for $S(T_1)$

$\Rightarrow$ S not continuous at T_1 $\Rightarrow$ $\left(\frac{\partial G}{\partial T}\right)_{p,N}$ is not well-defined at $T = T_1$ (or $T = T_2$ would be identical)

$\Rightarrow$ G not differentiable with respect to T @ $\begin{cases} T = T_1 \\ T = T_2 \end{cases}$

So a continuous fct can be non-differentiable but differentiable fcts <u>have to be</u> continuous.

<u>Some properties of continuous functions</u> ($f(x), g(x)$):

- if $f(x)$ is continuous, then if λ is a scalar ($\in \mathbb{R}$) constant $\rightarrow$ (*) $h(x) = \lambda f(x)$ is continuous as well

- if $h(x) = \lambda f(x) + \mu g(x)$, λ & μ are constants then $h(x)$ is continuous as well

- if (*) is true, then $\lambda = -1 \Rightarrow h(x) = -f(x)$ & $0 = h(x) + f(x)$ is also continuous

Sounds a bit like vectors, right?

if $\vec{V}_1$ vector, $\vec{V}_2 = \lambda \vec{V}_1$, λ scalar, $\vec{V}_2$ is a vector that lives in space with same # of dimensions as $\vec{V}_1$

- if $\vec{V}_1, \vec{V}_2 \in \mathbb{R}^n$ vectors in n-dimensions

$\vec{V}_3 = \lambda \vec{V}_1 + \mu \vec{V}_2$ (λ, μ scalars $\in \mathbb{R}$) is another vector

- if $\lambda = -1$ & $\vec{V}_2 = \lambda \vec{V}_1 \Rightarrow \vec{V}_2 = -\vec{V}_1$

& $\vec{V}_3 = \vec{V}_1 + \vec{V}_2 = \vec{0}$ in that case.

<u>Vectorial space</u> (VS)

Intuitively, a vectorial space is a structure that contains vectors & obeys certain rules concerning how one can manipulate these vectors.

- mathematically a vectorial space (VS) is a space where if u, v are elements (vectors) & λ, μ scalars (numbers)

  - $(\lambda + \mu) u = \lambda u + \mu u$
  - $u + v = v + u$
  - $(\lambda \mu) u = \lambda (\mu u)$
  - there is an element (vector) $0 = u - u$ & by extension every u admits an opposite $-u$

VS are also provide an inner product (scalar product)

$$\vec{u} \cdot \vec{v} = \lambda$$, where for example vectors $\vec{u}, \vec{v} \in \mathbb{R}^n$ & $\lambda \in \mathbb{R}$

take for example $\vec{u} = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix}$; $\vec{v} = \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix}$

$$\vec{u} \cdot \vec{v} = u_1 v_1 + u_2 v_2 + u_3 v_3 = \sum_j u_j v_j = \lambda$$

Why does it matter to us with continuous functions $f(x), g(x)$? Let's define the space of all continuous functions $\mathcal{C}^0$

$f : \mathbb{R} \longrightarrow \mathbb{R}$
$g : \mathbb{R} \longrightarrow \mathbb{R}$ (the same will be true for $f : \mathbb{R}^n \longrightarrow \mathbb{R}^n$)

if $\lambda, \mu \in \mathbb{R}$ are constants.

The space $\mathcal{C}^0$ is a vectorial space, because we can sum $f(x) + g(x)$ and multiply by scalars λ, μ to show that $\mathcal{C}^0$ satisfies all the conditions of a vectorial space.

What about the inner product ? (A sense of metric (magnitude) for "vectors").

$$\langle f, g \rangle_{a,b} = \int_a^b f(x)\, g(x)\, dx$$ is the scalar product over the interval $[a ; b]$ in $\mathcal{C}^0$

Same as your favorite vectors $\vec{u}, \vec{v}$ ...

if $\vec{u}\cdot\vec{v}$ $(= \langle \vec{u},\vec{v}\rangle) = 0$ then $\vec{u}$ is orthogonal to $\vec{v}$

well if $\langle f,g\rangle_{a,b} = 0$ $\Rightarrow$ f, g are said to be orthogonal

Vectorial basis:

In a vectorial space, we can define (not unique) a set (minimal) of vectors that allow us to reconstruct any vectors by multiplication with scalars & addition.

For instance a set of vectors $\vec{V}_1, \dots, \vec{V}_N$ $(\in \mathbb{R}^n)$ constitutes a vectorial basis of $\mathbb{R}^n$ if

- Any vector $\vec{u} \in \mathbb{R}^n$ can be written as

$$\vec{u} = \lambda_1\vec{V}_1 + \lambda_2\vec{V}_2 + \dots = \sum_{j=1}^{N} \lambda_j \vec{V}_j$$

with $\lambda_1, \dots, \lambda_N$ scalars $(\in \mathbb{R})$

- & $\vec{V}_1, \vec{V}_2, \dots$ are linearly independent

i.e $\sum_j \lambda_j \vec{V}_j = \vec{0}$ only if $\lambda_1 \dots \lambda_N = 0$

Some notes here

(i) the # of vectors that belong to a vectorial basis is equal to the dimension of the vectorial space.

in $\mathbb{R}^3$ $\hat{x}, \hat{y}, \hat{z}$ form a basis

r, θ, φ (spherical coordinates)

r, θ, z (cylindrical " ")

(ii) if vectors in the basis are orthogonal to each other $\langle \vec{v}_i, \vec{v}_j \rangle = 0 \quad i \neq j$

if $\vec{u} = \sum_{j=1}^{N} \lambda_j \vec{v}_j$, then $\lambda_j = \langle \vec{u}, \vec{v}_j \rangle$

Coefficients λ_j are projection of $\vec{u}$ onto $\vec{v}_j$.

<u>Back to our continuous functions and vectorial space $\mathcal{C}^0$</u>

Let's think about bases (non-unique) to write down these continuous functions

$$f(x) = \sum_j \lambda_j v_j(x)$$

$v_j(x)$ is a continuous function $v_j : x \in \mathbb{R} \mapsto v_j(x) \in \mathbb{R}$

- How many linearly independent fcts $v_j(x)$ do you need to span $\mathcal{C}^0$? (Dimension of $\mathcal{C}^0$)

What if $v_j(x) = x^j$ let's consider $x \in [0,1]$ a subspace of $\mathbb{R}$

$$\sum_{j=0}^{n} a_j \underbrace{x^j}_{v_j(x)} = 0$$ only if a_j are all $= 0$

$\Rightarrow$ linearly independent!

that means that x^{n+1} can't be written as a linear combination $\sum_{j=0}^{n} a_j x^j$

there is an infinite # of functions $v_j(x) = x^j$ that are all linearly independent of $v_k(x)$, $k \neq j$

$\Rightarrow$ Dimension of $\mathcal{C}^0(\mathbb{R})$ is infinite

$\Rightarrow$ Basis of $\mathcal{C}^0(\mathbb{R})$ requires an infinite # of elements

Some famous examples of vectorial bases for $\mathcal{C}^0(\mathbb{R})$:

A. Taylor expansion series:

$$f(x) = \sum_{k=0}^{\infty} a_k \, g_k(x) \qquad , \quad g_k(x) = x^k$$

$$a_0 = f(0)$$

$$a_1 = \left(\frac{df}{dx}\right)_{x=0} \quad ; \quad a_2 = \frac{1}{2}\left(\frac{d^2 f}{dx^2}\right)_{x=0}$$

$$a_k = \frac{1}{k!}\left(\frac{d^k f}{dx^k}\right)_{x=0}$$

$\Rightarrow$ polynomial basis $g_k(x)$

$$f(x) = f(0) + \underbrace{\left.\frac{df}{dx}\right|_{x=0} x}_{\substack{1^{st}\text{ order} \\ \text{"correction"}}} + \underbrace{\frac{1}{2}\left.\frac{d^2 f}{dx^2}\right|_{x=0} x^2}_{2^{nd}\text{ order}} + \ldots \quad \ldots$$

well intuition is simple here, if x is divided on both sides

$$\frac{f(x) - f(0)}{x} = \left.\frac{df}{dx}\right|_{x=0} + \frac{1}{2}\left.\frac{d^2 f}{dx^2}\right|_{x=0} x + \ldots \quad O(x^2)$$

as $x \to 0$ (limit

limit: $$\lim_{x\to 0} \frac{f(x)-f(0)}{x} = \underbrace{\lim_{x\to 0} \left.\frac{df}{dx}\right|_{x=0}}_{= \left.\frac{df}{dx}\right|_{x=0}} + \underbrace{\lim_{x\to 0}\left[\left.\frac{d^2f}{dx^2}\right|_{x=0} x + O(x^2)\right]}_{\to 0}$$

Definition of derivative

Taylor series: predicting $f(x)$ from $x_0=0$ $f(x_0=0)$ requires only slope at $x_0=0$ if $x \to x_0 = 0$ but if $x - x_0 \to 0$ "fast enough", then need higher correction terms (quadratic ...) to improve accuracy of $f(x)$

Another idea for bases is to decompose a function into simple periodic functions with different "frequencies"

here frequency $\to$ wavelength if x represents lengthscale / position

$\to$ angular frequency or period if x refers to time

B. <u>sine & cosine series</u>

$$f(x) = \sum_{k=0}^{\infty} a_k\, g_k(x)$$

$$g_k(x) = \sin(\pi k x) \text{ or } \cos(\pi k x)$$

Let's start with the cosine fct as a possible basis for $\mathcal{C}^0(\mathbb{R})$.

First, $\cos(x)$ is continuous for $x \in \mathbb{R} \Rightarrow \in \mathcal{C}^0(\mathbb{R})$

$\Rightarrow \cos(\pi k x)$ for $k = 0, 1, \ldots \in \mathcal{C}^0(\mathbb{R})$,

Actually, $\frac{d\cos(x)}{dx} = -\sin(x)$ & $\frac{d\sin(x)}{dx} = \cos(x)$

so $\cos(x) \in \mathcal{C}^\infty(\mathbb{R}) \Rightarrow$ infinitely continuous & differentiable.

- Can we build a basis with $\cos(\pi k x)$ for $\mathcal{C}^0(\mathbb{R})$?

$\Rightarrow$ they would need to "span" the whole space $\mathcal{C}^0(\mathbb{R})$, i.e. there exist a_k's such that

$$f(x) = \sum_k a_k \cos(\pi k x) \quad \text{for any } f(x) \in \mathcal{C}^0(\mathbb{R})$$

is that true?

$\Rightarrow$ No .... only even functions $\mathcal{C}^0_E(\mathbb{R}) \subset \mathcal{C}^0(\mathbb{R})$

$$\cos(-x) = \cos(x) \Rightarrow f(x) = \sum_k a_k \cos(\pi k x)$$
$$= f(-x) \ !$$

So $\cos(\pi k x)$, $k = 0, 1, \ldots$ can form a basis potentially for even-continuous fcts $\in \mathcal{C}^0(\mathbb{R})$

that subspace is also infinite in dimension.

Orthogonality of $\cos(\pi k x)$ for different k's.

$$I_{k,k'} \equiv \langle \cos(\pi k x), \cos(\pi k' x) \rangle \equiv \int_{-1}^{1} \cos(\pi k x)\cos(\pi k' x)\,dx$$

is the scalar product

(takes 2 functions $f(x), g(x) \to \mathbb{R}$ and yields a scalar value)

$$I_{k,k'} = 2\int_0^1 \cos(\pi k x)\cos(\pi k' x)\,dx \qquad \text{(even fcts)}$$

what if $k = k' = 0$?

$$I_{0,0} = 2\int_0^1 dx = 2$$

if $k = k' \neq 0$

$$I_{k,k} = 2\int_0^1 \cos^2(\pi k x)\,dx$$

use

$$\cos\alpha\cos\beta = \frac{1}{2}\left[\cos(\alpha-\beta) + \cos(\alpha+\beta)\right]$$

$$\Rightarrow \cos^2(\pi k x) = \frac{1}{2}\Big[\underbrace{\cos(0)}_{1} + \cos(2\pi k x)\Big]$$

$$I_{k,k} = 1 + \int_0^1 \cos(2\pi k x)\,dx = 1 + \underbrace{\frac{1}{2\pi k}\sin(2\pi k x)\Big|_0^1}_{0}$$

$I_{k,k'} = 1$ for any $k = k' \neq 0$

what if $k \neq k'$

$$I_{k,k'} = 2\int_0^1 \cos(\pi k x)\cos(\pi k' x)\,dx = \frac{2}{2}\int_0^1 \left[\cos(\pi(k-k')x) + \cos(\pi(k+k')x)\right]$$

$$= \int_0^1 \cos(\pi(k-k')x)\,dx + \int_0^1 \cos(\pi(k+k')x)\,dx$$

$$= \frac{1}{\pi(k-k')}\sin(\pi(k-k')x)\Big|_0^1 + \frac{1}{\pi(k+k')}\sin(\pi(k+k')x)\Big|_0^1 = \underline{\underline{0}}$$

$\Rightarrow$ $\cos(\pi k x)$ is orthogonal to $\cos(\pi k' x)$ if $k \neq k'$!

$\Rightarrow$ <u>orthogonal basis</u>

That is great because we can now easily compute coefficients a_k from $f(x)$

If $\quad f(x) = \sum_k a_k \cos(\pi k x)$

$$f(x)\cos(\pi k' x) = \sum_k a_k \cos(\pi k x)\cos(\pi k' x)$$

$$\int_{-1}^{1} f(x)\cos(\pi k' x)\,dx = \sum_k a_k \underbrace{\int_{-1}^{1}\cos(\pi k x)\cos(\pi k' x)\,dx}$$

$$= \delta_{k,k'} \equiv \begin{cases} 0 & \text{if } k = k' \\ 1 & \text{otherwise.} \end{cases}$$

or 2 if $k' = k = 0$

$\Rightarrow$ from orthogonality of $\cos(\pi k x)$

$$\Rightarrow \boxed{a_k = \int_{-1}^{1} f(x) \cos(\pi k x)\, dx}$$

Similarly for odd functions $f(x)$

$$f(x) = \sum_k a_k \sin(\pi k x)$$

$\sin(\pi k x)$ form orthogonal basis with

$$a_k = \int_{-1}^{1} f(x) \sin(\pi k x)\, dx$$

An example using the sine ~~expansion~~ series to solve a differential equation

Let's take a diffusion equation (more later on those...)

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2}$$ with initial condition $u(x, t=0) = f(x)$

& boundary conditions:

$u(0,t) = 0$

$u(1,t) = 0$

assume $$u(x,t) = \sum_{k=1}^{\infty} a_k(t) \sin(k\pi x)$$

First comment: that choice satisfies boundary conditions

$$\frac{\partial u}{\partial t} = \sum_{k=1}^{\infty} \frac{da_k}{dt} \sin(k\pi x)$$

$$\frac{\partial u}{\partial x} = \sum_{k=1}^{\infty} k a_k \cos(k\pi x)$$

$$\frac{\partial^2 u}{\partial x^2} = -\sum_{k=1}^{\infty} k^2 a_k \sin(k\pi x)$$

our PDE then looks like

$$\sum_{k=1}^{\infty} \frac{da_k}{dt} \sin(k\pi x) = -D \sum_{k=1}^{\infty} k^2 a_k \sin(k\pi x)$$

$$\sum_{k=1}^{\infty} \left[\frac{da_k}{dt} + k^2 D a_k \right] \sin(k\pi x) = 0$$

Orthogonality of $\sin(x)$ .... multiply by $\sin(k'\pi x)$

$$\sum_{k=1}^{\infty} \left[\frac{da_k}{dt} + k^2 D a_k \right] \sin(k\pi x) \sin(k'\pi x) = 0$$

$\int_{-1}^{1}$

$$\frac{da_{k'}}{dt} + k'^2 D a_{k'} = 0$$ that is true for all k'

$$a_{k'} = A_k \exp(-k'^2 D t)$$

$$a_{k'}(t=0) = A_k$$

$$u(x,t=0) = \sum_{k=1}^{\infty} A_k \sin(k\pi x) = f(x)$$

Solving for A_k

$$f(x) = \sum_{k=1}^{\infty} A_k \sin(k\pi x)$$

Same trick

$$f(x)\sin(k'\pi x) = \sum_{k=1}^{\infty} A_k \sin(k\pi x)\sin(k'\pi x)$$

$$\int_{-1}^{1} f(x)\sin(k'\pi x)dx = A_{k'}$$

$$\boxed{u(x,t) = \sum_{k=1}^{\infty} A_k \exp(-k^2 D t)\sin(k\pi x) \quad \text{with} \quad A_k = \int_{-1}^{1} f(x)\sin(k\pi x)\,dx}$$

- Fourier series

No problem for odd or even ~~~~ functions, but limited to periodic functions. If $f(x)$ is a periodic function, we can combine sine & cosine series to build

$$f(x) = \frac{a_0}{2} + \sum_{k=1}^{\infty} a_k \cos(k\pi x) + b_k \sin(k\pi x)$$

where again a_k's and b_k's can be retrieved using orthogonality of both bases.