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1.1 Some Random Calculus

In this section I will cover some basic calculus concepts which will be used in the later chapters. I start with the Divergence theorem

Theorem 1.1 — Divergence theorem. Let $F: \mathbb{R}^3 \to \mathbb{R}^3$ be a vector field defined on $\Omega \subset \mathbb{R}$. Then

$$\int_{\Omega} \nabla \cdot F dV = \int_{\partial \Omega} F \cdot d\vec{s}$$

By letting $F = \varphi \nabla \psi$, the theorem above helps us to define a similar notion to integration by parts in higher dimensions. To see this, first observe that

$$\nabla \cdot \varphi \nabla \psi = \nabla \varphi \cdot \nabla \psi + \varphi \underbrace{\nabla^2 \psi}_{\nabla \cdot (\nabla \psi)}.$$

You can check this by simply writing the equation term by term. Then the divergence theorem for $\varphi \nabla \psi$ will be

$$\int_{\Omega} \nabla \cdot (\varphi \nabla \psi) dV = \int_{\Omega} (\nabla \varphi \cdot \nabla \psi + \varphi \nabla^2 \varphi) dV = \int_{\partial \Omega} \varphi \nabla \psi \cdot d\vec{s}.$$

By rearranging the terms we will have

$$\int_{\Omega} \nabla \varphi \cdot \nabla \psi dV = \int_{\partial \Omega} \psi \nabla \varphi \cdot d\vec{s} - \int_{\Omega} \varphi \nabla \cdot (\nabla \varphi) dV$$

. To make this identity more similar to the integration by parts in 1D, let $F = \nabla \psi$. Then we will have the following theorem

Theorem 1.2 — Integration by parts in higher dimensions. Let $F : \mathbb{R}^3 \to \mathbb{R}^3$ be a vector field, and $\varphi : \mathbb{R}^3 \to \mathbb{R}$ an scalar function, both defined on Ω . Then

$$\int_{\Omega} (F \cdot \nabla \varphi) dV = \int_{\partial \Omega} \varphi F \cdot d\vec{s} - \int_{\Omega} \varphi \nabla \cdot F dV.$$

By applying the divergence theorem on $F = \psi \nabla \varphi - \varphi \nabla \psi$, and using the identity $\nabla \cdot (\psi \nabla \varphi) = \nabla \psi \cdot \nabla \varphi - \psi \nabla^2 \psi$, we can derive the Green's second identity.

Theorem 1.3 — Green's second identity. Let $\varphi, \psi : \mathbb{R}^3 \to \mathbb{R}$ defined on some region Ω . Then

$$\int_{\Omega} (\psi \nabla^2 \varphi - \varphi \nabla^2 \psi) dV = \int_{\partial \Omega} (\psi \nabla \varphi - \varphi \nabla \psi) \cdot d\vec{s}.$$

1.2 Some Random Linear Algebra

Definition 1.1 — Self adjoint matrix. A matrix $M:V\to V$ is self adjoint if and only if and only if

$$\langle v, Mu \rangle = \langle Mv, u \rangle$$

for $v, u \in V$. In words, $M = M^* = (\overline{M})^T$.

Proposition 1.1 The set of all basis sets for a vector space V is identical with the set of all non-singular and self-adjoint operators $M:V\to V$ up to matrix similarity

Proof. This is not a formal proof, but an informal discussion of the idea. Every self-adjoint matrix has a set of orthogonal eigenvectors that can be considered as a basis. \Box

1.3 Classification of The Second Order PDEs

Partial differential equations relate the partial derivatives of a function to each other. For example f can be a function of spacial coordinates (like x, y, z in the case of Cartesian coordinates), dynamical variable (like time), or any other kind of variables (like the space of genotypes g). For example suppose that $\Phi(x, y)$ represents the electric potential of a point charge. Such function should satisfy the Laplace equation:

$$\partial_{xx}\Phi + \partial_{yy}\Phi = 0.$$

Note that the symbols ∂_{xx} and ∂_{yy} are short symbols for $\frac{\partial^2}{\partial x^2}$ and $\frac{\partial^2}{\partial y^2}$ respectively.

Definition 1.2 Order of PDE The order of a PDE is the highest derivative that occurs in the equation.

Based on the definition above, the Laplace equation is a second order partial differential equation.

There are three categories of the second order PDEs that every other type of a second order PDE can be converted to one of these kinds. The most general type of a second order PDE can be written as:

$$A\partial_{xx}u + B\partial_{xy}u + C\partial_{yy}u + D\partial_{x}u + E\partial_{y}u + Fu = k$$
(1.3.1)

In which the coefficients are all a function of x, y (but not u in which case the PDE will be nonlinearx). Equation 1.3.1 can be summarized in a more compact form using the derivative operator L:

$$Lu=0$$
,

in which:

$$L = A\partial_{xx} + B\partial_{xy} + C\partial_{yy} + D\partial_x + E\partial_y + F$$

Because of the similarities of the equation 1.3.1 with the generic quadratic equation describing the conic sections, we call each class of second order PDEs with its corresponding conic section. The generic equation describing the conic sections is:

$$Ax^{2} + Bxy + Cy^{2} + Dx + Ey + K = 0. {(1.3.2)}$$

All of the conic sections (ellipse, parabola, hyperbola) can be described with the equation 1.3.2 which is determined with the discriminant $\Delta = B^2 - 4AC$. for $\Delta = 0$, $\Delta > 0$, and $\Delta < 0$ the conic section will be **parabolic**, **hyperbolic**, and **elliptic** respectively. Table 1.1 summarizes special categories of the linear second order PDEs that frequently occur in physical applications.

1.3.1 Intuitive Derivation of the Second Order PDEs

The three classes of the second order linear PDEs in table 1.1 can be derived intuitively using the continuity law (conservation law) and the constitutive law that is determined by the nature of the problem which is the subject of the following sections.

PDE	Analogous conic sec.	Δ	Class	Application
$u_t = u_{xx}$	$T = x^2$	0	parabolioc	Diffusion - Heat Equation
$u_{tt} = u_{xx}$	$T^2 = x^2$	$\Delta > 0$	Hyperbolic	Wave Equation
$u_{xx} + u_{yy} = 0$	$x^2 + y^2 = 0$	$\Delta < 0$	Elliptic	Laplace
$u_{xx} + u_{yy} = c$	$x^2 + y^2 = k$			Poisson

Table 1.1: A summary of the three class of second order linear PDE.

The most important part of deriving the PDE equations is the continuity law or conservation law. This fact is imposed because of our common sense about nature. Suppose that we want to study the concentration of of a red ink in a infinitesimal cube. The continuity equation, in simple terms, state that the change of the concentration of the ink inside the infinitesimal cube is equal to the ink that has entered the cube from outside from its boundaries (we are assuming no source or sink of ink inside the cube). For instance, consider the infinitesimal box in figure 1.3.2. The change of the concentration of the ink inside the cube is $\frac{\partial c}{\partial t}$. Because we know that there are no sources or sinks of ink inside the cube, then the change in the concentration is equal to the amount that comes in and goes out from the boundaries of the box. To put this in numbers, we introduce the important vector quantity $flux \Phi$. Flux is the amount of particles flow per unit area per unit time (see figure 1.3.1).

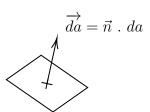


Figure 1.3.1: The dot product $\overrightarrow{\Phi}.\overrightarrow{da}$ is the amount of particles passing through the infinitesimal cross section in unit time.



Figure 1.3.2: The infinitesimal cube for deriving the continuity equation

Let's get back to the infinitesimal cube in figure 1.3.2 and derive the continuity equation. We can start we tracking the net change in the number of particles inside the cube due to the flux in x direction:

$$-\frac{dN_x}{dt} = \Phi_x(x, y, z).(-dzdy) + \Phi_x(x + dx, y, z).(dzdy)$$
$$= (\Phi_x(x + dx, y, z) - \Phi_x(x, y, z))dydz$$

Note that the negative sign in the LHS of the equation above is simply to match the meaning of the two sides of the equations. For instance, if the RHS of the equation above is positive, it means that the net change of the number of particles in the box in negative (meaning that particles are leaving the box) which is equivalent to $-\frac{dN}{dt}$. Similarly in the y and z direction:

$$-\frac{dN_y}{dt} = (\Phi_y(x, y + dy, z) - \Phi_y(x, y, z))dxdz$$
$$-\frac{dN_z}{dt} = (\Phi_z(x, y, z + dz) - \Phi_z(x, y, z))dxdy$$

So the net change in the number of particle in the box per dt will be:

$$-\frac{dN}{dt} = -\left(\frac{dN_x}{dt} + \frac{dN_y}{dt} + \frac{dN_z}{dt}\right)$$

$$= (\Phi_x(x + dx, y, z) - \Phi_x(x, y, z))dydz +$$

$$(\Phi_y(x, y + dy, z) - \Phi_y(x, y, z))dxdz +$$

$$(\Phi_z(x, y, z + dz) - \Phi_z(x, y, z))dxdy$$

By dividing the both sides of the above equation by the volume of the cube dV = dxdydz we can write:

$$\frac{dc}{dt} = -(\partial_x \Phi_x + \partial_y \Phi_y + \partial_z \Phi_z) = -\nabla \cdot \Phi$$

In which c = N/V is the concentration, ∇ is the divergence operator, and Φ is the flux.

Definition 1.3 Continuity Equation The following important relation is known as the continuity equation (or conservation law):

$$\frac{dc}{dt} + \nabla \cdot \Phi = 0 \tag{1.3.3}$$

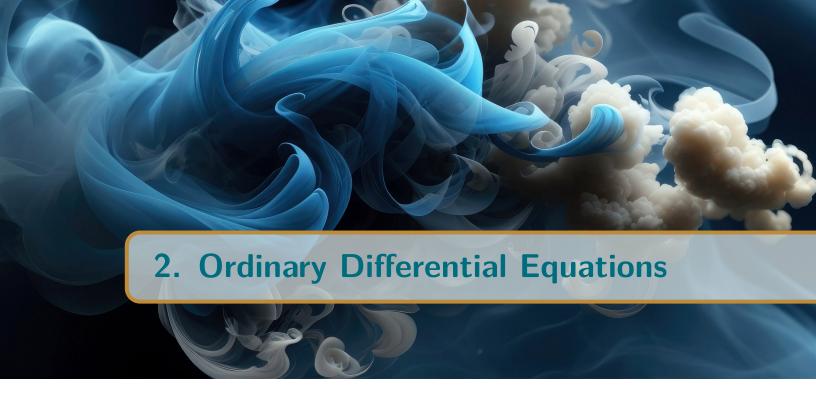
in which Φ is the flux, c is the concentration, and ∇ is the divergence operator.

will be used to derive the wave equation

1.3.2 Constitutive Laws: Advection, Diffusion and Wave Equation

Having the continuity equation in hand makes the derivation PDEs very straight forward. We only need to insert the constitutive laws (which are enforced by the nature of the problem) in the continuity equations derived in the section above.

- Fick's Law \rightarrow Constitutive law for diffusion
- Hook's law \rightarrow Constitutive law for the wave equation



Let's start by studying the following first order differential equation for u

$$u' + mu = f, (1)$$

where $m \in \mathbb{R}$ and $f : \mathbb{R} \to \mathbb{R}$ is a continuous function. In fact, we are trying to find a function that its derivative plus some constant times the function itself produces the function f. One way to tackle this problem is to multiply both sides by e^{mx} . Then, we will get

$$e^{mx}u' + mue^{mx} = fe^{mx}, \quad x \in \mathbb{R}.$$

Now the trick is to do a similar thing as completing the square in algebra, with only difference that we are aiming at completing the derivative. In other words

$$(e^{mx}u(x))' = f(x)e^{mx}, \quad x \in \mathbb{R}.$$

Now by integrating both sides (or, equivalently, using the fundamental theorem of calculus) we will get

$$e^{mx}u(x) - u(0) = \int_0^x f(s)e^{ms}ds.$$

By a little rearrangement of the terms we will get

$$u(x) = ce^{-mx} + \int_0^1 f(s)e^{m(s-x)}ds, \quad c \in \mathbb{R}$$

Now we can see that on only there is one function that satisfies that particular relation imposed by the differential equation, there is in fact a continuum of functions satisfying the differential equations that are parameterized by $c \in \mathbb{R}$. It turns out that the set of all such functions, as a set, has some very interesting properties. Let's

call this set \mathcal{A} . As we discussed above, the elements of this set is parameterized by $c \in \mathbb{R}$. We can also specify this set as

$$\mathcal{A} = \{ u \mid u(x) = ce^{-mx} + \int_0^x f(s)e^{m(s-x)}ds \ \forall c \in \mathbb{R} \}$$

Note that we will assume that the function f is Lipschitz continuous. Then we will be sure that all of the possible solutions of the ODE above are in set A. Studying this set more closely, reveals the fact that this set is actually a linear space, or, a vector space. This is true since

- (A1) $u, v \in \mathcal{A} \implies u + v = v + u \in \mathcal{A}$.
- (A2) $\forall u, v, r \in \mathcal{A}$ we have u + (v + r) = v + (u + r).
- (A3) $\mathcal{O} \in \mathcal{A}$ such that $v + \mathcal{O} = \mathcal{O} + v = v$ for all $v \in \mathcal{A}$.
- (A4) $\forall v \in \mathcal{A}, \exists u \in \mathcal{A} \text{ s.t. } v + u = u + v = \mathcal{O}.$
- (M1) $\forall v \in \mathcal{A}$ we have $\mathcal{I} \cdot v = v \cdot \mathcal{I} = v$.
- (M2) $\forall v \in \mathcal{A}$ we have $\mathcal{O} \cdot v = v \cdot \mathcal{O} = \mathcal{O}$
- (M3) $\forall v \in \mathcal{A}, \ a, b \in \mathbb{R} \text{ we have } a(bv) = (ab)v$
- (D1) $\forall u, v \in \mathcal{A}, \ a \in \mathbb{R} \text{ we have } a(u+v) = au + av.$
- (D2) $\forall u \in \mathcal{A}, \ a, b \in \mathbb{R} \text{ we have } (a+b)u = au + bu.$

Proof. All of the properties of this set follows immediately from the fact that \mathbb{R} is a vector space. To see this, see the following proof for (A1). Let $u, v \in \mathcal{A}$. Then $\exists c_1, c_2 \in \mathbb{R}$ such that

$$u(x) = c_1 e^{-mx} + \int_0^x f(s)e^{m(s-x)}ds, \quad v(x) = c_2 e^{-mx} + \int_0^x f(s)e^{m(s-x)}ds.$$

Thus

$$(u+v)(x) = (c_1+c_2)e^{-mx} + \int_0^x f(s)e^{m(s-x)}ds.$$

Since $c_1 + c_2 \in \mathbb{R}$, then $u + v \in \mathcal{A}$.

So far, we have fined a set of functions \mathcal{A} that solves the differential equation. However, now, we can ask for more requirement. For instance, we can ask for functions that satisfy certain initial conditions, i.e. $u(0) = u_0$. Or we can ask for functions that are defined on some interval, say [0,1] that satisfy certain boundary conditions like u(0) + u'(1) = 3, or u(0) = u(1), etc. For the case of specifying an initial condition, say $x(0) = x_0$, we can find a unique $x \in \mathcal{A}$ that solves the ODE and satisfies this initial value problem (choose $x \in \mathcal{A}$ that has $c = x_0$).

Be Careful Here ' Consider the following initial value problem

$$\dot{x} = x^{2/3}, \qquad x(0) = 0.$$

Then at any open interval that the function x(t) does not take the value 0, we can write the ODE as

$$\frac{\dot{x}}{x^{2/3}} = 1.$$

Now by integration we get the set of all solutions of the ODE

$$\mathcal{A} = \{x : [a, b] \to \mathbb{R} : x(t) = (\frac{x+c}{3})^3, \ x(t) \neq 0 \ \forall t \in [a, b]\}.$$

Clearly, the constant solution $x(t) \equiv 0$ doe not belong to the set \mathcal{A} . However, we can easily verify that $x(t) \equiv 0$ is a solution to the initial value problem. So when the function f is not descent enough (not Lipschitz continues in this case), then the set \mathcal{A} does not contain all of the solutions for the initial value problem. So in conclusion, the initial value problem has two solutions $x(t) = t^3/3$ that belongs to \mathcal{A} and $x(t) \equiv 0$ which is not in \mathcal{A} .

However, if the function f (RHS of the initial value problem) is Lipschitz continuous, then by the Picard iteration argument we can show that there is always a unique solution that can be achieved by the integration^a.

 $^a\mathrm{see}$ the chapter 1 of the book "Ordinary Differential Equations: Qualitative Theory" by Barreira.

However, in the case of specifying boundary conditions (boundary condition problems), like demanding u(0) = u(1) the situation is not as clear as the initial value problem. Given that the RHS function is Lipschitz continuous and all of the solutions of the ODE lives in the set \mathcal{A} , then our task is basically look for functions in \mathcal{A} (which is basically isomorphic to \mathbb{R}) to see which of them satisfy the boundary condition. Then we might find no solutions, or a unique solution, or more than one solution (note the similarity with finding the solutions of a linear system AX = B that based on the characterizations of the matrix A we might have different scenarios for the solutions.)

Back to our example above, we find that the solutions of

$$u' + mu = f$$

are all in the set

$$\mathcal{A} = \{ u \mid u(x) = ce^{-mx} + \int_0^x f(s)e^{m(s-x)}ds \ \forall c \in \mathbb{R} \}$$

So we can determine which functions in A satisfies our boundary condition. This

leads to the following equation

$$c = ce^{-m} + \int_0^1 f(s)e^{m(s-1)} ds,$$

which implies

$$c = \frac{1}{1 - e^{-m}} \int_0^1 e^{m(s-1)} f(s) \ ds, \qquad m \neq 0.$$

Thus when $m \neq 0$, we have a unique function in \mathcal{A} that satisfies the boundary condition. However, when m = 0, then the above equation does not make sense. Then the function $u \in \mathcal{A}$ where

$$u(x) = c + \int_0^x f(s) \ ds.$$

To satisfy the boundary condition, we need to have

$$u(0) = u(1) \implies c = c + \int_0^1 f(s)ds \implies \left[\int_0^1 f(s) ds = 0\right].$$

So in the case where m=0, if $\int_0^1 f(s)ds=0$, then we have infinitely many solutions for the boundary value problem. But if $\int_0^1 f(s)ds \neq 0$, then there is no solutions for the boundary value problem.

Summary 2.1 Consider the following ODE

$$u' + mu = f$$
.

where f is Lipschitz continuous. Then the set of all solutions to this ODE is

$$\mathcal{A} = \left\{ u \mid u(x) = ce^{-mx} + \int_0^x f(s)e^{m(s-x)}ds \ \forall c \in \mathbb{R} \right\}.$$

Then for any initial value $u(0) = u_0$, we can find a unique $u \in \mathcal{A}$ that satisfies the initial value problem $(c = u_0)$. However, for the boundary value problem u(0) = u(1) we will have the following cases

• $m \neq 0$. Then there is a unique $u \in \mathcal{A}$ where

$$c = \frac{1}{1 - e^{-m}} \int_0^1 e^{m(s-1)} f(s) \ ds$$

• m = 0. Then there are two cases

- $-\int_0^1 f(s)ds = 0$. We will have infinite number of solutions $\forall c \in R$ for the BVP.
- $-\int_0^1 f(s)ds \neq 0$. We will have no solutions for BVP.

We can think about the boundary value problem in a more systematic way. First note that all the functions $u:[0,1] \to \mathbb{R}$ that satisfies the boundary condition u(0) = u(1) for a vector space (easy to check). Thus we can think about our boundary value condition in the following way

Let $\mathcal{B} = u : \mathcal{C}^1([0,1],\mathbb{R}) : u(0) = u(1)$ be a Banach space. This is a linear space equipped with the norm $||u|| = \max\{||u||_{\infty}, ||u'||_{\infty}\}$ (thus \mathcal{B} is a Hilbert space). Let $Y = \mathcal{C}([0,1],\mathbb{R})$ equipped with the suprimum norm. Consider for any $m \in \mathbb{R}$, the linear operator $L_m : X \to Y$ define as $L_m u = u' + mu$. Given any $f \in Y$ find those $u \in \mathcal{B}$ such that $L_m u = f$.

If we have a unique solution, then we can write $u = L_m^{-1} f$ where L_m^{-1} is the inverse operator of L_m . So the uniqueness of the solution is the question invertibility of the operator L_m . This operator is the inverse of a differential operator, thus it is an integral operator. For the specific example that we solved above, we can easily calculate this integral operator.



In my opinion, Green's function is nothing other than expressing the solution of a problem in a nice and clean way. So I would say it acts more like a level of abstraction thing that helps to express the solution of a particular problem in a special way that can be used for more higher level thinking for further development, that otherwise would be very hard. I other words, I believe Green's function is basically looking at a solution from a different perspective. I know that all of these statements are pretty wage, but you might get some kind of similar feeling after reading this chapter!

3.1 Green's function in linear algebra

Consider the following linear equation

$$Mu = f$$

where M is a symmetric $n \times n$ matrix with $\det(M) \neq 0$, and $u, v \in \mathbb{R}^n$. Our problem is to find u given the known matrix M and f. The most simple way to approach this problem is basically

$$u = M^{-1}f.$$

To be honest, this is not a solution at all! This expression literally stating Mu = f in an equivalent way. It is basically saying the vector u can be calculated by the act of the inverse mapping M^{-1} on the input function f. Now we can seek different ways to find this inverse mapping, which we are not discussing here.

Instead, we are going to discuss another very simple approach, that turns out the be generalization to infinite dimensional spaces as well! The strategy is basically utilizing the fact that every non-singular symmetric function defines a natural set of orthogonal basis vectors (which are actually the eigenvectors of the matrix)for the space. Let

$$\mathbb{B} = \{v_i\}_{i=1}^n$$

be the set of all normalized eigenvectors of M, which corresponding eigenvalues $\{\lambda_1, \lambda_2, \dots, \lambda_i\}$ (note that these eigenvalues need not to be all distinct). All these things wants to say that we have a unique factorization of every vector in the space in terms of these eigenvectors. So we can write

$$\vec{u} = \sum_{i=1}^{n} \hat{u}_i \vec{v}_i, \qquad \vec{f} = \sum_{i=1}^{n} \hat{f}_i \vec{v}_i.$$

Now, simply by substituting the terms in Mu = f, and matching the terms we will get

$$\hat{u}_i = \frac{\hat{f}_i}{\lambda_i}.$$

Voila! we solved the system of equations, and the solution basically is

$$\vec{u} = \sum_{i=1}^{n} \frac{\hat{f}_i}{\lambda_i} v_i.$$

At this stage, you might finish you job and head towards the home being proud of yourself in solving this problem. But, we can do just a little bit modification to the expression above and view things from a different angle, which turns out the be very useful when considering certain problems in infinite dimensions (like ODEs and PDEs). We know that the coefficients \hat{f}_i are basically the projection of the vector f on the basis vector v_i . I.e. $\hat{f}_i = \langle v_i, f \rangle = \sum_{k=1}^n (v_i)_k f_k$. Let's insert this in the equation above

$$\vec{u} = \sum_{i=1}^{n} \frac{1}{\lambda_i} (\sum_{k=1}^{n} (v_i)_k f_k) v_i.$$

or

$$\vec{u} = \sum_{i=1}^{n} \sum_{k=1}^{n} \frac{(v_i)_k v_i}{\lambda_i} f_k \implies \boxed{\vec{u} = \sum_{i=1}^{n} \sum_{k=1}^{n} G_{i,k} f_k}.$$

Where I call matrix G the Green's matrix! By staring at the equation above, you will find out that matrix G has a very simple structure.

Note that the eigenvectors are assumed to be normalized.