Chapter 1

Introduction

1.1 Fundamentals

1.1.1 Scalar Field vs Vector Field

A *scalar field* is a zero tensor field which associates a scalar value to every point in a space-possibly physical space. The scalar may be any dimensionless mathematical number or a physical quantity. Mathematically, a scalar field on a region $\mathfrak{U}$ is a real or complex-valued function or distribution on $\mathfrak{U}$. The region $\mathfrak{U}$ may be a set in some Euclidean space, Minkowski space or more generally a subset of a manifold. The scalar field can be *continuous* or *discontinuous* depending on the kind of restrictions applied to it. Examples of a scalar field includes temperature, pressure or humidity field in a room.

A *vector field* is a first order tensor field which assigns a vector to each point in a subset of space. A vector is a geometric object that has a magnitude and a direction attached to a point, and is represented by arrows. Vector fields are often used to model, for example the speed and direction of a moving fluid through space or the strength and direction of a magnetic force as it changes from one point to another.

1.1.2 Vector fields on subsets of Euclidean space

Let's assume a vector field is represented by a vector-valued function $V : S \to \mathbb{R}^n$ in standard Cartesian coordinates $(x_1, \ldots, x_n)$, in a subset $\mathfrak{S}$ in $\mathbb{R}^n$. V is a continuous vector field if each component of V is continuous, and V is a C^k vector field if each component of V is k times continuously differentiable. A vector field can be visualised as attaching a vector to individual points within an n-dimensional space.

Consider a real valued C^k-function f defined on $\mathfrak{S}$ and two C^k-vector fields $V,\ W$ also defined on $\mathfrak{S}$, then the two operations scalar multiplication and vector addition

$$\begin{aligned}(fV)(p) &\coloneqq f(p)V(p)\\ (V+W)(p) &\coloneqq V(p)+W(p)\end{aligned} \tag{1.1}$$

define the module of C^k-vector fields over the ring of C^k-functions where the multiplication of function is defined pointwise.

1.1.3 Vector fields on manifolds

A vector field on a manifold $\mathfrak{M}$ assigns a vector in tangent space $T_p(\mathfrak{M})$ for every $p \in \mathfrak{M}$. Elaborating more, a vector field F is a mapping from $\mathfrak{M}$ into the tangent bundle $T_p(\mathfrak{M})$ so that $p \cdot F$ is the identity mapping where p denotes the projection from $T_p(\mathfrak{M})$ to $\mathfrak{M}$

Another definition of a vector field is: Consider a smooth vector field X on a manifold $\mathfrak{M}$ which is a linear map $X : C^\infty(\mathfrak{M}) \to C^\infty(\mathfrak{M})$ such that:

$$X(fg) = fX(g) + X(f)g \qquad \forall\, f, g \in C^\infty(\mathfrak{M}) \tag{1.2}$$

1.2 Basic Objects

1.2.1 Interpolation

Interpolation is a method of constructing new data points within the range of known discrete set of data points. Various interpolation methods are often used to represent any function at more data points than already available. There are many interpolation methods available but we will mainly focus on the multivariate interpolation methods. Multivariate interpolation refers to the interpolation on functions of more than one variable.

Linear Interpolation

Linear inteprolation is a method of curve fitting using linear polynomials to construct new data points within the range of a discrete set of known data points. If we know the data points, for instance $(x_0, f_0), \ldots, (x_n, f_n)$ then the value at any point (x, f), such that $x_i \leq x \leq x_{i+1}$ can be found as:

$$x = x_i + \alpha(x_{i+1} - x_i) \tag{1.3}$$

where, $\alpha = \frac{x - x_i}{x_{i+1} - x_i}$, $\alpha \in [0, 1]$, then

$$f(x) = (1 - \alpha)f_i + \alpha f_{i+1} \tag{1.4}$$

Bilinear Interpolation

Extending the above concept, bilinear interpolation is useful when we want to interpolate a function of two variables on a rectilinear grid. As the name suggests, the key idea is to perform two linear interpolations, first in one direction, followed by other in another direction.

Consider a set of data points in a cell with points $(x_i, y_i, f(x_i, y_i))$, $(x_{i+1}, y_i, f(x_{i+1}, y_i))$, $(x_i, y_{i+1}, f(x_i, y_{i+1}))$, and $(x_{i+1}, y_{i+1}, f(x_{i+1}, y_{i+1}))$ as shown below.

Therefore, to calculate the value at position $f(x, y)$

$$\begin{aligned} f(x, y) &= (1 - \beta)[(1 - \alpha)f_{i,j} + \alpha f_{i+1,j}] + \beta[(1 - \alpha)f_{i,j+1} + \alpha f_{i+1,j+1}] \\ &= (1 - \beta)f_j + \beta f_{j+1} \end{aligned} \tag{1.5}$$

with

$$\begin{aligned} f_j &= (1 - \alpha)f_{i,j} + \alpha f_{i+1,j} \\ f_{j+1} &= (1 - \alpha)f_{i,j+1} + \alpha f_{i+1,j+1} \end{aligned} \tag{1.6}$$

with local coordinates

$$\alpha = \frac{x - xi}{x_{i+1} - x_i}, \qquad \beta = \frac{y - y_i}{y_{i+1} - y_i}, \qquad \alpha, \beta \in [0, 1] \tag{1.7}$$

Thus, solving further we get

$$f(x, y) = (1-\alpha)(1-\beta)f_{i,j} + \alpha(1-\beta)f_{i+1,j} + (1-\alpha)\beta f_{i,j+1} + \alpha\beta f_{i+1,j+1} \tag{1.8}$$

Trilinear Interpolation

Analogous to above definition, trilieanr interpolations are used when there are three variables. It's similar to making linear interpolations with respect to each variable once. We will directly look at the formula as the derivation is same as above:

$$\begin{aligned} x_d &= \frac{x - x_0}{x_1 - x_0} \\ y_d &= \frac{y - y_0}{y_1 - y_0} \\ z_d &= \frac{z - z_0}{z_1 - z_0} \end{aligned} \tag{1.9}$$

Interpolating in the x-direction first

$$\begin{aligned} f_{00} &= f_{000}(1 - x_d) + f_{100}x_d \\ f_{01} &= f_{001}(1 - x_d) + f_{101}x_d \\ f_{10} &= f_{010}(1 - x_d) + f_{110}x_d \\ f_{11} &= f_{011}(1 - x_d) + f_{111}x_d \end{aligned} \tag{1.10}$$

Now, in y-direction

$$\begin{aligned} f_0 &= f_{00}(1 - y_d) + f_{10}y_d \\ f_1 &= f_{01}(1 - y_d) + f_{11}y_d \end{aligned} \tag{1.11}$$

and now finally in z-direction

$$f = f_0(1 - z_d) + f_1 z_d \tag{1.12}$$

1.2.2 Differentiation of a vector

The derivative of a vector function $\mathbf{a}(p)$ of a single parameter p is

$$\dot{\mathbf{f}}(x) = \lim_{\delta x \to 0} \frac{\mathbf{f}(x + \delta x) - \mathbf{f}(x)}{\delta x} \tag{1.13}$$

If we write $\mathbf{a}$ in terms of components relative to a fixed coordinate system as $\mathbf{f} = (f_1, f_2, f_3)$, then

$$\dot{\mathbf{f}}(x) = \left(\frac{\mathrm{d}f_1}{\mathrm{d}x}, \frac{\mathrm{d}f_2}{\mathrm{d}x}, \frac{\mathrm{d}f_3}{\mathrm{d}x} \right) \tag{1.14}$$

Finite Difference Method

Finite-Difference Methods are numerical methods used to obtain the derivatives in order to solve differential equations. The finite differences, i.e. $f(x+b) - f(x+a)$ is approximated to the derivatives by dividing it by $b-a$. Mathematically, it's written as:

$$\Delta f(x) = \dot{f}(x) = \frac{f(x+b) - f(x+a)}{b-a} \tag{1.15}$$

There are three types of finite differences methods:

1. **Forward Differences**: This method uses the values of $f(x+h)$ and $f(x)$ to calculate the derivatives. It gives the error accuracy of order $\mathcal{O}(h)$. Mathematically, it is expressed as:

$$\Delta f(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h} \tag{1.16}$$

2. **Backward Differences**: As the name signifies, this method uses the values of $f(x)$ and $f(x-h)$ to calculate the derivatives. It also gives the error accuracy of order $\mathcal{O}(h)$. Mathematically, it is expressed as:

$$\Delta f(x) = \lim_{h \to 0} \frac{f(x) - f(x-h)}{h} \tag{1.17}$$

3. **Central Difference**: This method uses the values of $f(x + \frac{1}{2}h)$ and $f(x - \frac{1}{2}h)$ to calculate the derivatives. It's a rather more reliable method as it provides the error accuracy of order $\mathcal{O}(h^2)$. Mathematically, it is expressed as:

$$\Delta f(x) = \lim_{h \to 0} \frac{f(x + \frac{1}{2}h) - f(x - \frac{1}{2}h)}{h} \tag{1.18}$$

1.2.3 Integration of a vector

The integration of a vector function of a single scalar variable can be considered as the opoosite of differentiation. It's expressed as:

$$f(x) = \int \dot{f}(x)\,\mathrm{d}x \tag{1.19}$$

1.2.4 Line integrals through fields

Line integrals are the integrated development of a field as it moves through a defined path. We know that the definition of an integral for a scalar function *f(x)* of a single scalar variable x is defined as:

$$\int f(x)dx = \lim_{\substack{n\to\infty \\ \delta x_i\to 0}} \sum_{i=1}^{n} f_i \delta x_i \tag{1.20}$$

A *vector line integral* is the integration of the vector field along a curve, i.e. to determine it's line integral. The line integral is constructed similar to Riemann Integral and it exists if the vector field is continuous and the curve has finite length. There are three types of integrals, depending on the nature of product:

1. Integrand $U(\mathbf{r})$ is a vector field, hence the integral is a vector.

$$\mathbf{I} = \int_L U(\mathbf{r})\,\mathrm{d}\mathbf{r} \tag{1.21}$$

2. Integrand $\mathbf{a}(\mathbf{r})$ is a vector field with a dot product with $\mathrm{d}\mathbf{r}$ hence the integral is a scalar

$$I = \int_L \mathbf{a}(\mathbf{r}) \cdot \mathrm{d}\mathbf{r} \tag{1.22}$$

3. Integrand $\mathbf{a}(\mathbf{r})$ is a vector field with a cross product with $\mathrm{d}\mathbf{r}$ hence the integral is a vector

$$\mathbf{I} = \int_L \mathbf{a}(\mathbf{r}) \times \mathrm{d}\mathbf{r} \tag{1.23}$$

1.2.5 Surface Integrals

Analogous to line integrals, the surface integral is calculated by dividing the surface S into infinitesimal vector elements of area $\mathrm{d}\mathbf{S}$, where the direction of the vector $\mathrm{d}\mathbf{S}$ represents the direction of the surface normal and its magnitude representing the area of the element. It's just the generalisation of the multiple integration to integration over surfaces.

For a surface $\mathbf{S} = (x.y)$, surface integral is calculated as:

$$\iint_S f(x,y)\,\mathrm{d}\mathbf{S} = \iint_S f(x,y)\,\mathrm{d}x\,\mathrm{d}y \tag{1.24}$$

Similar to above case of line integrals, there are three possibilities here as well:

1. $\int_S U \, \mathrm{d}\mathbf{S}-$ scalar field U; vector integral.
2. $\int_S \mathbf{a} \cdot \mathrm{d}\mathbf{S}-$ vector field $\mathbf{a}$; scalar integral.
3. $\int_S \mathbf{a} \times \mathrm{d}\mathbf{S}-$ vector field $\mathbf{a}$; vector integral.

1.2.6 Volume Integrals

Volume integral refers to an integral over a 3-dimensional domain. Analogous to above cases, volume integral is taken as the limit of a sum of products as the size of the volume element tends to zero. Mathematically,

$$\iiint_V f(x, y, z) \, \mathrm{d}\mathbf{V} = \iiint_V f(x, y, z) \, \mathrm{d}x \, \mathrm{d}y \, \mathrm{d}z \tag{1.25}$$

One obvious difference is that element of volume is a scalar. Similar possibilities here are:

1. $\int_V U(\mathbf{r}) \, \mathrm{d}V-$ scalar field; scalar integral.
2. $\int_V \mathbf{a} \, \mathrm{d}V-$ vector field; vector integral.

1.3 Differential Operators

Vector calculus has three main differential operators namely *gradient, divergence* and *curl* which are defined on scalar or vector fields. These operators use the del operator (∇), also known as nabla. Let's look at these operators one by one.

1.3.1 Gradient

A gradient is a multi-variable generalisation of the derivative. It symbolises the direction of greatest ascent or descent for a function as it represents the slope of the tangent of a function. The magnitude of the gradient is equal to the slope of the tangent in the direction of greatest rate of increase of the function.

Given a function $f(x_1, x_2, \ldots, x_n)$, the gradient of a scalar function is represented by ∇f and for a vector function as $\vec{\nabla} f$. It is often also denoted as grad f. Thus mathematically, gradient of f is defined as the unique vector field whose dot product with any unit vector $\mathbf{v}$ at each point x is the directional derivative of f along $\mathbf{v}$, i.e.

$$(\nabla f(x)) \cdot \mathbf{v} = D_{\mathbf{v}} f(x) \tag{1.26}$$

If $f : \mathbb{R}^n \rightarrow \mathbb{R}$ at a point x in $\mathbb{R}^n$ is a linear map from $\mathbb{R}^n \rightarrow \mathbb{R}$, then for any v in $\mathbb{R}^n$ the derivative or gradient of f at x can be written as:

$$(\nabla f(x))_x \cdot \mathbf{v} = df_x(v) = \begin{bmatrix} \frac{\mathrm{d}f}{\mathrm{d}x_1} \\ \frac{\mathrm{d}f}{\mathrm{d}x_2} \\ \vdots \\ \frac{\mathrm{d}f}{\mathrm{d}x_n} \end{bmatrix}^T \tag{1.27}$$

Jacobian Matrix

Let's also introduce the another very important concept, i.e. *Jacobian Matrix.* Jacobian matrix is the matrix of all first-order partial derivatives of a vector-valued function. It generalises the derivative of a scalar-valued function of multiple variables. In other words, it's a gradient of a scalar-valued function of multiple variables. It can be considered of as expressing imposition of transformation which causes of stretching, rotation or transforming.

Suppose $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$ is a function which gives the output as the vector $\mathbf{f}(x) \in \mathbb{R}^m$ from the input vector $\mathbf{x} \in \mathbb{R}^n$. Then, the Jacobian matrix $\mathbf{J}$ of $\mathbf{f}$ is an $m \times n$ matrix defined as:

$$\mathbf{J} = \begin{bmatrix} \dfrac{\partial \mathbf{f}}{\partial x_1} & \cdots & \dfrac{\partial \mathbf{f}}{\partial x_n} \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\mathrm{d}x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix} \tag{1.28}$$

or, component-wise:

$$\mathbf{J}_{ij} = \frac{\partial f_i}{\partial x_j} \tag{1.29}$$

The matrix is also denoted by D$\mathbf{f}$, $\mathbf{J}_{\mathbf{f}}$ and $\frac{\partial(f_1,\ldots,f_m)}{\partial(x_1,\ldots,x_n)}$.

1.3.2 Divergence

A divergence is a vector operator which gives the quantity of a vector field's source at each point, thus producing a scalar field. More elaboration, the divergence represents the volume density of the outward flux of a vector field from an infinitesimal volume around a point.

Let's consider an example to have a better intuition. Consider velocity of air at each point which is being heated or cooled. When the air is cooled, it contracts in all directions, and velocity field points inwards. Thus, the divergence of velocity has a negative value. On the other hand, when the air heated, it expands in all directions and the velocity field points outwards from the region. Thus, the divergence has a positive value.

Thus, it can be concluded that the divergence of a vector field represents the flux generation per unit volume at each point of the field. Mathematically, divergence is defined by:

$$\operatorname{div} \mathbf{F} = \nabla \cdot \mathbf{F} = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right) \cdot (F_1, F_2, F_3) = \frac{\partial F_1}{\partial x} + \frac{\partial F_2}{\partial y} + \frac{\partial F_3}{\partial z} \tag{1.30}$$

1.3.3 Curl

Curl is a vector operator which defines infinitesimal rotation of a vector field in 3-dimensional Euclidean space. It takes a vector field as input and produces another vector field. The attributes of this generated vector i.e. length and direction tell us about the rotation at that point. The axis of rotation defines the direction of the curl and the magnitude of rotation defines curl's magnitude. The curl of a irrotational vector field is zero.

In simpler terms, the circulation of any vector $\mathbf{F}$ around any closed curve C is defined as $\oint_C \mathbf{F} \cdot d\mathbf{r}$ and the curl of the vector field $\mathbf{v}$ represents the vorticity, or circulation per unit area, of the field. Thus it measures the density of angular momentum of the vector flow at a point, i.e. the amount to which the flow circulates around a fixed axis.

Curl of a vector field is represented as $\nabla \times \mathbf{F}$. If $\mathbf{F}$ is composed as

$[F_x, F_y, F_z]$, then mathematically

$$\begin{aligned}\nabla \times \mathbf{F} &= \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ F_x & F_y & F_z \end{vmatrix} \\ &= \left(\frac{\partial F_z}{\partial y} - \frac{\partial F_y}{\partial z}\right)\mathbf{i} + \left(\frac{\partial F_x}{\partial z} - \frac{\partial F_z}{\partial x}\right)\mathbf{j} + \left(\frac{\partial F_y}{\partial x} - \frac{\partial F_x}{\partial y}\right)\mathbf{k}\end{aligned} \tag{1.31}$$

1.3.4 Laplacian

Laplace operator or the Laplacian denoted by $\nabla \cdot \nabla, \nabla^2, or \Delta$ is a differential operator which is given by the divergence or the gradient of a function on Euclidean space. The Laplacian $\Delta f(x)$ of a function f at point x is the rate at which the average value of f over spheres centered at x deviates from *f(x)* as the radius of the sphere grows. In a cartesian coordinate system, the Laplacian is given by the sum of second partial derivatives of the function with respect to each individual variable.

The Laplacian expresses the flux density of the gradient flow of a function. For instance, Laplacian of the chemical concentration at a point can be defined as the net rate at which a chemical dissolved in a fluid moves toward or away from that point. The Laplacian operator is also used for ridge detection which we will study later.

As defined already that the Laplacian operator is the second order differential operator in the n-dimensional Euclidean space, defined as the divergence $(\nabla \cdot)$ of the gradient (∇f). It maps C^k functions to C^{k-2} functions for $k \geq 2$, i.e. $\Delta : C^k(\mathbb{R}^n) \to C^{k-2}(\mathbb{R}^n)$. Thus, if f is a twice-differentiable real-valued function, the Laplacian of f is defined by:

$$\Delta f = \nabla^2 f = \nabla \cdot \nabla f \tag{1.32}$$

where $\nabla = \left(\frac{\partial}{\partial x_1}, \ldots, \frac{\partial}{\partial x_n}\right)$. Therefore, the Laplacian of f is the sum of all the unmixed second partial derivatives in the Cartesian coordinates x_i:

$$\Delta f = \sum_{i=1}^{n} \frac{\partial^2 f}{\partial x_i^2} \tag{1.33}$$

1.3.5 Vector Laplacian

The vector Laplacian operator, denoted by ∇^2 is analogous to the scalar Laplacian as seen above. It is a differential operator which is defined over a vector field. Scalar Laplacian when applied to a scalar field returns a scalar quantity, similarly vector Laplacian when applied to a vector field returns a vector quantity.
The vector Laplacian of a vector field $\mathbf{F}$ is defined as:

$$\nabla^2\mathbf{F} = \nabla(\nabla \cdot \mathbf{F}) - \nabla \times (\nabla \times \mathbf{F}) \tag{1.34}$$

In Cartesian coordinates, it's reduced to an easier form as:

$$\nabla^2\mathbf{F} = (\nabla^2 F_x, \nabla^2 F_y, \nabla^2 F_z) \tag{1.35}$$

1.4 Integral Theorems

The three basic vector operators have corresponding theorems which generalises the fundamental theorem of calculus to higher dimensions:

1.4.1 Gradient theorem

The gradient theorem, also called the fundamental theorem of calculus for line integrals, explains that the line integral through a gradient field can be measured by evaluating the original scalar field at the endpoints of the curve.

Mathematically, let's assume $\phi : U \subseteq \mathbb{R}^n \to \mathbb{R}$ and γ is any curve from $\mathbf{x}$ to $\mathbf{y}$. Then

$$\phi(\mathbf{y}) - \phi(\mathbf{x}) = \int_{\gamma[\mathbf{x},\mathbf{y}]} \nabla\phi(\mathbf{r}) \cdot \mathrm{d}\mathbf{r} \tag{1.36}$$

The gradient theorem implies that the line integrals are path independent when evaluated through gradient fields. The inverse, i.e. any path-independent vector field can be expressed as the gradient of a scalar field, also holds true.

1.4.2 Divergence theorem

The divergence theorem, also known as Gauss's theorem relates the vector flux through a surface to the behaviour of the vector field inside the surface. A more sophisticated explaination is that the divergence theorem equates the volume integral of the divergence over the area inside the surface to the outward flux of a vector field through a closed surface.

As an example let's consider a fluid in some area with sources and sinks. Then the divergence theorem states that the sum of rate of fluid flow through all the sources and sinks is equal to the net flux out of a region.

Mathematically, if we assume a volume V which is a subset of $\mathbb{R}^n$ and it's smooth boundary S, and $\mathbf{F}$ is a continuously differentiable vector field defined on the neighbourhood of V, then the divergence theorem states:

$$\iint_V (\nabla \cdot \mathbf{F})\,\mathrm{d}V = \oiint_S \mathbf{F} \cdot \mathbf{n}\,\mathrm{d}S \tag{1.37}$$

where, $\mathbf{n}$ is the outward pointing unit normal field of the boundary ∂V. The left side of the integral is over the volume V whereas the right side is over the boundary of V.

1.4.3 Curl theorem

Curl theorem relates a line integral around a closed path to a surface integral over what is called a capping surface of the path. It is a theorem on $\mathbb{R}^3$

Let $\gamma : [a, b] \to \mathbb{R}^2$ be a piecewise smooth non-intersecting continuous loop in the plane, such that γ divides $\mathbb{R}^2$ into two components, a compact one and a non-compact. Let D denote the compact part which is bounded by γ and $\psi : D \to \mathbb{R}^3$ is smooth, with $S := \psi(D)$. If Γ is the space curve defined by $\Gamma = \psi(\gamma(t))$ and $\mathbf{F}$ is a smooth vector field on $\mathbb{R}^3$, then:

$$\oint_\Gamma \mathbf{F} \cdot \mathrm{d}\Gamma = \iint_S \nabla \times \mathbf{F} \cdot \mathrm{d}\mathbf{S} \tag{1.38}$$

1.5 Fluid Flows

There are two ways to describe fluid flows:

I **Lagragian approach**: Lagrangian approach is the way of observing the fluid motion where the observer follows an individual fluid parcel as it travels through space and time. In simpler terms, the individual particles are "marked" and their positions, velocities etc. are described as a function of time. The physical laws such as Newton's laws and conservation of mass and energy laws are directly applied to each individual particle. This can be thought of as sitting in a car and going along a road.

II **Eulerian approach**: Eulerian approach is a way of looking at fluid motion which instead focuses on specific locations in the space through which the fluid flows with time evolution. Here, the individual particles are not identified, but instead a control volume is defined. Each property of the fluid is expressed as a field which is a function of space and time.

Thus, Eulerian view doesn't care about the location or velocity of any particular particle but rather the properties of whatever particle is present at a particular location at the time of interest. An example would be sitting on roadside and watching cars pass by from the fixed location. Since fluid flow is a continuum phenomenon, at least down to the molecular level, the Eulerian description is usually preferred in fluid mechanics.

In the Eulerian specification of a field, it is represented as a function of a position $\mathbf{x}$ and time t. For instance, the flow velocity is represented as a function $\mathbf{u}(\mathbf{x}, t)$ On the other hand in Lagrangian field of view, the individual particles are tracked over time. The fluid parcels are labelled by some time-independent vector field $\mathbf{x}_0$. The flow is described by a function $\mathbf{X}(\mathbf{x}_0, t)$ providing the position of parcel $\mathbf{x}_0$ at time t.
Therefore, two specifications can be related as:

$$\mathbf{u}(\mathbf{X}(\mathbf{x}_0, t), t) = \frac{\partial \mathbf{X}}{\partial t}(\mathbf{x}_0, t) \tag{1.39}$$

1.5.1 Material Derivative

Material derivative relates the kinematics and dynamics of the Lagrangian and Eulerian specifications. Suppose we have a floe field $\mathbf{u}$, and we know a generic field with Eulerian specification $\mathbf{F}(\mathbf{x}, t)$. The total rate of change of $\mathbf{F}$ in a specific flow parcel is computed as:

$$\frac{\mathrm{D}\mathbf{F}}{\mathrm{D}t} = \frac{\partial \mathbf{F}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{F} \tag{1.40}$$

where ∇ denotes the gradient with respect to $\mathbf{x}$ and operator $\mathbf{u} \cdot \nabla$ is applied to each component of $\mathbf{F}$. The above relation shows that the total rate of change of fucntion **F** as the fluid parcels travels through a flow field described by its Eulerian specification **u** is equal to the sum of the local rate of change and convective rate of change pf **F**.

1.5.2 Field Lines

A field line is a locus that is defined by a vector field and a starting location within the field. Field lines are important for visualizing the vector fields which are otherwise hard to imagine. A field line for a vector field is constructed by tracing a path through space that follows the direction of vector field.Technically, the path should be differentiable at all interior points and the tangent line to the path at each point should be parallel to the vector of the field at that point.
In a fluid flow, there are four kind of feld lines namely streamlines, streaklines, pathlines and timelines. They differ from each other when the flow changes with time, i.e. an unteady flow. In a flow streamlines and streaklines never intersect but pathlines are allowed to intersect themselves. The reason will be clear as we look each line in more detail.

Streamlines

Streamlines represent a family of curves that are instantaneously tangent to the velocity vector of the flow. If we consider a massless fluid element, then streamlines show the direction in which they travel at any point in time.

Streamlines are mathematically defined as:

$$\frac{\mathrm{d}\vec{x}_S}{\mathrm{d}s} \times \vec{u}(\vec{x}_S) = 0 \tag{1.41}$$

where $\vec{x}_S(s)$ is the parametric representation of one streamline at one moment in time and $\vec{u}(\vec{x}_S)$ is velocity at the point. If the components of the velocity are $\vec{u} = (u, v, w)$ and those of the streamline as $\vec{x}_S = (x_s, y_s, z_s)$, we deduce

$$\frac{\mathrm{d}x_s}{u} = \frac{\mathrm{d}y_s}{v} = \frac{\mathrm{d}z_s}{w} \tag{1.42}$$

which thus depicts that the curves are infact parallel to velocity field. Thus, streamline is a solution of the initial value problem of an ordinary differential equation:

$$\begin{cases} \frac{\mathrm{d}\vec{x}_S}{\mathrm{d}s} = \vec{u}(\vec{x}_S) \\ \vec{x}(0) = \vec{x}_0 \end{cases} \tag{1.43}$$

Streamlines are calculated instantaneously that means that they are calculated from an instantaneous flow velocity field at a particular instance of time. Since a particle a fluid particle cannot have two different velocities at the same point, that's why different streamlines at the same instant in a flow don't intersect.

Pathlines

Pathlines are the trajectories that individual fluid particles follow. It can be thought of as following the path of a fluid element in the flow over a certain period. It can be thought of as the path taken by the particle which can be determined by a series of streamlines at different continuous moments in time.

Mathematically, pathlines are defined as:

$$\begin{cases} \frac{\mathrm{d}\vec{x}_P}{\mathrm{d}t}(t) = \vec{u}_P(\vec{x}_P(t), t) \\ \vec{x}_P(t_0) = \vec{x}_{P_0} \end{cases} \tag{1.44}$$

The suffix P indicates that we follow the motion of a fluid particle. The velocity is calculated at the position $\vec{x}_P$ of the particle at time t and the curve is parallel to the flow velocity vector $\vec{u}$.

Streaklines

Streaklines are the loci of points of all the fluid particles that have passed continuously through a particular spatial point in the past. in simpler words, it connects the particles released at same position during time interval. An example of streakline is a trace of dye that is released into the floe at a fixed position.

Streaklines can be represented as:

$$\begin{cases} \frac{\mathrm{d}\vec{x}_P}{\mathrm{d}t} = \vec{u}_P(\vec{x}_P, t) \\ \vec{x}_P(t = \tau_P) = \vec{x}_{P_0} \end{cases} \tag{1.45}$$

where, at location $\vec{x}_P$ and time t, the velocity of particle P is $\vec{u}_P$. The parameter τ_P parameterizes the streakline $\vec{x}_P(t, \tau_P)$ and $0 \leq \tau_P \leq t_0$, where t_0 is a time of concern.

Timelines

Timelines are formed by propagation of a line of massless elements in time. The idea is to connect particles that are released simultaneously along a curve. More precisely, these are the lines formed by a set of fluid particles that were marked at a previous instant in time, creating a line or a curve with the propagation of particles that is displaced in time.

Chapter 2

Dynamical Systems

2.1 Introduction

Dynamical system is a mathematical model to represent a function that develops in time. It is defined as a set of $\{\mathfrak{M}, T, \mathfrak{D}\}$ where $\mathfrak{M}$ is the manifold, T is the one-dimensional directed space, and $\mathfrak{D}$ is an operator that maps $\mathfrak{M}$ onto itself. In simpler words, dynamical system at any particular time has a given state represented by a set of real numbers that can be characterised by a point in a phase space. Physically, it can be inferred that a dynamical system is an ensemble of particles whose state variables follow differential equations and vary with time as these equations involve time derivatives. Thus, for a particular time interval from a current state, only one future state is obtained, making the future deterministic.

The manifold $\mathfrak{M}$ is defined as the state space, the directed space T is time, and $\mathfrak{D}$ is the development equation or operator, defining how the state $\mathbf{u} \in \mathfrak{M}$ traverse through time. A state $\mathbf{u(t)}$ consisting of state variables describes the state of the system at time t which is obtained by applying the operator $\mathfrak{D}$ on the current state. Therefore, we only look at Markovian systems. Over time on applying the operator $\mathfrak{D}$ several successive states $\mathbf{u(t)}$ with $t \in T$ are obtained which form the trajectories in $\mathfrak{M}$Ṡuch solutions of the differential equations help us to understand various phenomenon in a more comprehensive manner by shifting the scale from microscopic level to a macroscopic level.

Typical examples of a dynamical system include oscillating pendulum, Lorenz 63.

2.2 Physical Point Mass

A simple dynamical system is a point mass that propagates through a physical space. Let $\mathbf{x}$ represents the position in some domain Ω and let $\mathbf{v}(\mathbf{x}$,t) represents the velocity,

$$\dot{\mathbf{x}} = \mathbf{v}(\mathbf{x}, t) \tag{2.1}$$

The point mass follows the trajectory, given as:

$$\mathbf{x}\,(t) = \mathbf{x}_0 + \int_0^t \mathbf{v}\,(\mathbf{x}(\tau), \tau)\,d\tau, \tag{2.2}$$

where $\mathbf{x}_0 = \mathbf{x}(0)$. Above equation is an example of development operator as it helps to obtain a future state $\mathbf{x}(t)$ from current state $\mathbf{x}_0$. In a sophisticated way, this can be represented as $\mathbf{x}(t) = \mathfrak{D}_t\mathbf{x}(0)$.

A trajectory can be understood as two different interpretations:

1. the path through which a point particle traverses from the start point defined by set of initial conditions, or

2. the set of points or states which can be reached from a particular point for $t > 0$ or set of particles from which the initial state can be achieved when going backwards in time i.e. $t < 0$.

Usually, considering the complexity that can arise with higher derivatives, only first order derivatives are considered. It has a twofold effect, firstly intuitively the interpretation is easier and secondly, in continuous cases the development equation always has a form such as (2.1). In case, equations with higher derivatives are defining the state space, effort is made to reduce the n^{th} order differential equation in a set of n first-order differential equation. For eg, if the dynamics of a mass point is defined as:

$$\ddot{\mathbf{x}} = \mathbf{a}(\mathbf{x}, t) \tag{2.3}$$

where, $\mathbf{x}$ denotes the position and $\mathbf{a}$ denotes the acceleration, the order of differential equation is reduced by increasing the number of equations, which is shown as follows:

$$\begin{aligned} \dot{\mathbf{x}} &= \mathbf{v}(\mathbf{x}, t) \\ \dot{\mathbf{v}} &= \mathbf{a}(\mathbf{x}, t) \end{aligned} \tag{2.4}$$

Thus, above method of reducing the order of differential equations by increasing the number of equations, emphasizes on the equivalence between order and dimension.

2.3 General Aspects of Dynamical System

Here, we proceed to define the different elements of dynamical system, namely state space or manifold $\mathfrak{M}$, time T and development operator $\mathfrak{D}$.

2.3.1 State Space

State space consists of a minimum set of variables which mathematically completely define the dynamical system at a time. These set of variables $\{u_1, \ldots, u_n\}$ are called state variables. The values of such a set of variables is known as the state of the system. And the set of all possible states is defined as the state space. We can group dynamical systems in different categories based on their structure of state space. The system can be low dimensional such as undamped pendulum with two state variable $\left\{\theta, \dot{\theta}\right\}$, the angle and it's derivative or of high dimensions such as n dimensional Lotka-Voltera equations. The system can be discrete, continuous, or hybrid. If the state takes values from a finite-set $\{u_1, \ldots, u_n\}$, then it's a discrete system. For eg. a light switch makes a discrete dynamical with two values, $\mathbf{u} \in \{ON,OFF\}$. A continuous system is defined when the state takes values from a Euclidean space $\mathbb{R}^n$ for some $n \geq 1$, as in the motion of a pendulum. A hybrid system has a part of the state taking value from finite set, while the other part is taking values from a $\mathbb{R}^n$ space. Using a computer to control the motion of a pendulum is one such example of a hybrid system.

2.3.2 Time

The order of states in a dynamical system is given by the orderly sequence of the time space. The future states of the system must be completely determined by the state variables at a given time. The evolution of states under time variable can be discrete or continuous. If the time is discrete, then the evolution of system takes place in discrete time steps, which are usually takes as integer values $t = 0, 1, \ldots$. The state of the system is thus defined at time t as $\mathbf{u}_t$. Many a times, a dynamical system is defined such that it takes as a state at time t and gives the output state at next time. Therefore, in cases where we start at state $\mathbf{u}_0 = \mathbf{u}(0)$, and feed the initial conditions to development operator, we obtain $\mathbf{u}_1 = \mathfrak{D}_0(\mathbf{u}_0)$ and subsequently obtain the sequence of states $\mathbf{u}_1, \mathbf{u}_2, \ldots$. Such a system where the states at all times are obtained by the development operator $\mathfrak{D}$ and initial condition $\mathbf{u}_0$ defines a dynamical system. On other hand, when the state evolves continuously through time, it's called as a continuous dynamical system. As time t evolves, the state of system evolves simultaneously through state space. The development operator thus defines how the state would evolve through time.

2.3.3 Development

Development of a system in most cases, is dependent on the current state of the system. In such models, sequence of states is achieved which are dependent only on the previous state. Such models follow, what is known as *Markov Processes.* Though in some cases, the following state might be also dependent on history of the system which blows up the dimensionality of the system, thus making it difficult to comprehend. Examples of such systems can be, when a rat stops falling in the trap after several iterations because it learned from historic events. For the sake of simplicity, in this thesis we only consider systems that are Markovian in nature.

Autonomous and Non-Autonomous Systems An *autonomous system* is a system which does not depend explicitly on the independent variable. In dynamical systems, an autonomous system is one where the development equation does not depend explicitly on time i.e. all system parameters are constant. Such a system is also known as *time-invariant systems.* On the other hand, a *non-autonomous system* itself changes with time, which is given by some time-dependent parameters and varying equations or rules.

A good example of an autonomous system is a simple undamped pendulum, where the underlying fundamental physics do not change with time. Another example could be the population of rabbits through centuries. Such a system can be represented with some differential equations consisting of several parameters. Now consider, that there is another parameter such as another invasive species which affect their population, and such a system becomes non-autonomous. if we also involve this parameter into the system, the system will change into autonomous again from non-autonomous system. Mathematically, this can be achieved by including the time as an additional state variable, such that state vector $\mathbf{u} = u_1, \ldots, u_n$ becomes $\mathbf{u} = u_1, \ldots, u_{n+1}$ where $u_{n+1} = t, \dot{u_{n+1}} = 1$, which increases the dimension of the system by 1.

Development Equation: Development equation defines the evolution of any dynamical system. On a broader classification, depending on the time, the system can be discrete or continuous.

Continuous systems: A continuous system is one where the state can be defined as any real number in a specific interval. In other words, it's a system where the state changes continuously over time. Typically, a continuous system is represented as:

$$\dot{\mathbf{u}} = f(\mathbf{u}) \tag{2.5}$$

with $f(\mathfrak{M}) \subset \mathfrak{M}$. Above equation, is a typical example of a *first-order ordinary differential equation (ODE).* Such ODEs can be solved by several numerical methods such as Euler Method, Runge-Kutta Method etc. For a fluid flow, often $\dot{\mathbf{u}}$ represents the velocity field in the phase space. An example of such a system is amount of liquid in a water tank.

Discrete Systems: Discrete system is one where the state takes a specific value from a subset of real numbers and often the states in between two states might not be defined. In other words, it's a system whose state is discrete and remains in a state for some time and then changes only at a time point. Such a system can be written as:

$$\mathbf{u}_{i+1} = f(\mathbf{u}_i) \tag{2.6}$$

where the index i is the discrete time step and f maps $\mathfrak{M}$ onto itself. Such system is also referred to as a map. An example of such a system is number of patients in a hospital on any particular day.

In discrete systems, since the time step is fixed, the development of a system based on numerical solution of ODE or PDE is usually different from the continuous system. For example, if we consider the population of rabbits in a limited environment, then during the mating season their population would increase, so from t_i to t_{i+1} the population would change from $\mathbf{u}_i$ to

$\mathbf{u}_{i+1}$. Now, consider that at t_{i+1}, there's a flood and the population decreases because of scarcity of food. Such a system with sudden changes is difficult to formalise as a continuous system with a set of ODEs or PDEs, and can only be easily understood as a discrete system.

State Variables vs Parameters: A development equation of a dynamical system consists of three parts- $\mathbf{u}$, $\mathbf{p}$ and $\mathbf{f}$, each focusing on several different aspects of the development of the system.

- A state variable $\mathbf{u}$ is one of the set of variables which are used to express the mathematical state of a dynamical system. The state of a system is describes the minimum essential factors needed to determine the future behaviour of the dynamical system when no external forces are acting on the system. The state variable represent the system's surficial appearance and typically varies rapidly. For example, concentration of some transported quantity or the density of a population.

- The parameters $\mathbf{p}$ tell the aspects of the system that are considered as the part of its setup or structure. They usually change on the time scales much bigger than the one of $\mathbf{u}$. One main reason to keep $\mathbf{p}$ different than $\mathbf{u}$ and $\mathbf{f}$ is that it helps the understand the impact of a changing environment on the dynamical system's development. Examples of parameters include the rates for the growth and interaction of populations.

- Finally, the function $\mathbf{f}$ represents the most persistent structures of a system, basically it's crux. Changing the function usually reflects the most on the development of the dynamical system.

2.4 One-Dimensional Continuous System

Here, we focus on a system whose state $\mathbf{u} \in \Omega \in \mathbb{R}$ is continuous in space and time and development is continuous in time. Hence, T is time, Ω represents the manifold $\mathfrak{M}$, and the development equation is given by:

$$\dot{\mathbf{u}} = f(\mathbf{u}) \tag{2.7}$$

Above equations can be solved using numerical solvers, such that a particular state is known and the states through which the system flows is obtained.

We define an *initial value problem (IVP)*, if an initial state or condition of the system such as $\mathbf{u}_0 = \mathbf{u}(0)$ is given and the later stages of development can be thus construed. On the other end, if we know the end conditions, then such a system is popularly called a *control problem.* Our focus will be on initial value problems.

2.4.1 Fixpoints and Stability

A fix point of a function, mathematically is defined as the element of the function's space which maps the function to itself. In simpler words, it means that if $f(u) = u$, then u is the fix point of the system. Similarly, for the initial state if $f(u) = 0$, then $\boldsymbol{u}_0 = \boldsymbol{u}(0)$ make the fix point of the system. A set of such fix points is called fixed set. For example, $f(u) = u^2 - 3u + 4$ has a fixpoint at $\mathbf{u} = 2$, as $f(2) = 2$. One key aspect which is often talked about is the stability of the fix points, i.e. how does the system develop when we look at $\boldsymbol{u}_0 \pm \varepsilon$, where ε is infinitesimal. The question of interest is, whether the fixpoint $\boldsymbol{u}_0$ attracts or repels the nearby trajectories. Thus, now we define the conditions for a fixpoint to be termed as attractor or repellor.

Attractors: An attractor or attractive fix $\boldsymbol{u}_0$ of a development operator $f(u)$ is such that for any value of u in the state space close to $\boldsymbol{u}_0$, the iterated development sequence $u, f(u), f(f(u)), f(f(f(u))), \ldots$ state converges to $\boldsymbol{u}_0$. When there's a small perturbation from $\boldsymbol{u}_0$ i.e.$\boldsymbol{u}_0 + \varepsilon$, then the sign of new state $f(\boldsymbol{u}_0) + \varepsilon$ is opposite to the sign of ε such that the state is pushed back to $\boldsymbol{u}_0$. Let's put the value of $\boldsymbol{u} = \boldsymbol{u}_0 + \varepsilon$ in the equation and do a Taylor expansion around $\boldsymbol{u}_0$, such that:

$$\dot{\varepsilon} = a\varepsilon + \mathcal{O}(\varepsilon^2), a = \frac{df}{du}|_{u=u_0} \tag{2.8}$$

On neglecting the higher order terms and integrating, we obtain:

$$\varepsilon(t) = \varepsilon_0 \exp(\sigma t) \tag{2.9}$$

where ε_0 is the initial perturbation, which leads to $\sigma = a$. Hence, fixpoint u_0 is stable if $a = d_u f(u)|_{u=u_0} < 0$.

Repellers: Repellers are the unstable fix points at which the value of $a > 0$ such that the sign of ε and $f(u_0 + \varepsilon)$ is same. Thereby, the trajectories around this point rapidly diverge to more stable areas because $\dot{u}$ pushes the states away from u_0. If we reverse the time, then attractor and repeller change their role and start behaving oppositely in retrospect.

Neutral Points: We have an attractor or a repeller as long as the first non-vanishing order of $f(u_0)$ is odd, but when the first non-vanishing order is even, we have a different scenario. In such cases, fixpoint has an attractive nature on one side and repulsive on other. Such points are called neutral points.

2.5 Multi-Dimensional Continuous Systems

Extending the beforementioned concepts, we can now consider a dynamical system with state variable $(u_1, u_2) \in \Omega$, manifold $\Omega \in \mathbb{R}^2$ and development equation:

$$\dot{u_1} = f_1(u_1, u_2) \tag{2.10}$$

$$\dot{u_2} = f_2(u_1, u_2) \tag{2.11}$$

where f_1 and f_2 are nonlinear functions. In a concise form with boundary conditions, it can be represented as:

$$\dot{u} = f(u) \tag{2.12}$$

2.5.1 Flows and Trajectories

Flow is a motion of particles in a medium. Mathematically, it can be defined as the temporal rate of change of the state of the system, in our case $\dot{u}$ which represents the system's velocity. The flow field is an affine function of position in the state space, defined as:

$$\dot{u} = f(u) = Au + b \tag{2.13}$$

where, , A is a matrix, b a vector of numbers and u the position vector.

The *trajectory* traces the motion of a single particle. Thus, a trajectory represents the development of the state of system with time from some initial state u_0

$$u(t) = u_0 + \int_0^t \dot{u}(u(\tau))d\tau \tag{2.14}$$

Usually, it's not easier to solve such equations analytically, therefore, we have to use more sophisticated tools to solve such equations like Euler method, Runge-Kutta etc. For $t > 0$, we get trajectories forward in time, i.e. trajectories for future states, and for $t < 0$, we get trajectories backward in time, i.e. trajectories for past states.

2.5.2 Fixpoints and Nullclines

Earlier, for one-dimensional systems, we described fixpoint as the state u_0, where the state satisfies the condition $f(u_0) = 0$. Extending this concept to multi-dimensions, we achieve what is known as nullclines in addition to the fixpoints. The nullcline of component i is defined as:

$$\mathbf{u} : \dot{u}_i = f_i(\mathbf{u}) = 0, \tag{2.15}$$

Nullclines are also known as zero-growth isoclines, where the set of points in the phase plane have zero first-order derivative. Therefore, the field through these points is either straight up or straight down. Nullclines thus separate the state space into different regions which exhibit varied characteristics. The fixpoints of a multi-dimension system exists where all the nullclines intersect, such that $\dot{u}_i = f_i(\mathbf{u}) = 0$. In a two-dimensional linear system, the nullclines are represented by two lines on a two-dimensional plot as shown:

2.5.3 Local Stability

Using the same concepts as of one-dimensional case, we again look at the neighbourhood of $\mathbf{u}_0$ with a small perturbation ε, such that $\mathbf{u} = \mathbf{u}^0 + \varepsilon$. On doing a Taylor's expansion on f, we obtain:

$$\dot{\mathbf{u}} = d_u(\mathbf{u}_0 + \varepsilon) = f(\mathbf{u}_0 + \varepsilon) \tag{2.16}$$

$$\dot{\varepsilon} = \mathbf{a}\varepsilon, \mathbf{a} = \begin{pmatrix} a_{11} & \cdots & a_{11} \\ \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{nn} \end{pmatrix}, a_{ij} = \frac{\partial f_i}{\partial u_j}|_{u=u_0} \tag{2.17}$$

where $\mathbf{a}$ is the Jacobian matrix. In the above formulation, ε is a vector and $\mathbf{a}$ is a matrix. There are various methods like singular value decomposition to do an eigen decomposition of any square matrix such as $\mathbf{a}$. The matrix $\mathbf{a}$ can be decomposed into three matrices, $\mathbf{a} = PDP^{-1}$, where P consists of eigenvectors of $\mathbf{a}$ and D is a diagonal matrix which contains the eigenvalues. From linear algebra, we know that an eigenvector or characteristic vector of a linear transformation is a non-zero vector that only changes by a scalar value when the linear transformation is applied to it. If the state space is finite-dimensional, then such linear transformation can be defined by square matrix. Thus, mathematically, we can write this as:

$$\mathbf{av} = \sigma \mathbf{v} \implies |\mathbf{a} - \sigma \mathbb{I}|\mathbf{v} = 0, \tag{2.18}$$

where $\mathbb{I}$ is an identity matrix, and $\mathbf{v}$ is an eigenvector with σ as its eigenvalue. Solving, det $|\mathbf{a} - \sigma \mathbb{I}|$ yields an n_{th} order polynomial solving which gives us n eigenvalues $\sigma_1, \ldots, \sigma_n$. On transforming (1) with the eigenbasis $\mathbf{v}_1, \ldots, \mathbf{v}_n$ of $\mathbf{a}$, gives us n independent linear differential equations:

$$\dot{\varepsilon}_i(t) = \sigma_i \varepsilon i, \tag{2.19}$$

where ε_i is the projection of ε onto the eigenvector . On integrating this, we come across the earlier result,

$$\sigma_i(t) = \varepsilon_{i_0} \exp(\sigma_i t) \tag{2.20}$$

where ε_{i_0} is the initial perturbation towards the direction of eigenvector i. Thus, as per prior discussion, it can be understood that fixpoint $\mathbf{u}_0$ is stable if for all $i, \Re(\sigma_i) < 0$ and unstable if $i, \Re(\sigma_i) > 0$. Now, we can define what's known as hyperbolic point, which is when the $i, \Re(\sigma_i) \neq 0, \forall i$. If atleast one sign is positive and one negative, we get a *hyperbolic saddle point*. If $\Re(\sigma_i) = 0$, we have to consider the higher order terms to say anything about such points. Thus, such points are called critical points.

Lyapunov Exponents and Deterministic Time Horizon

The eigensystem of $\mathbf{a}$ i.e. the set of eigenvectors is also useful to understand the stability in the direction of each eigenvector $\mathbf{v}_i$ in addition to overall stability of $\mathbf{u}_0$. Such a system characterises the rate of separation or fluctuation in any direction. Thus, it can be thought that the eigenvalue σ_i is the *Lyapunov exponent* in direction i. Mathematically, the *Lyapunov exponent* is defined as the rate of separation of infinitesimally close trajectories. Decomposing the ε into a sum of eigenvectors as $\varepsilon(t) = \sum_i \varepsilon_i \mathbf{v}_i$ and be the initial perturbation. Then, linear approximation gives:

$$\varepsilon(t) = \sum\nolimits_i \varepsilon_{i_0} \exp(\sigma_i t) \mathbf{v}_i \tag{2.21}$$

To calculate the development of small separation $\Delta\varepsilon$ between two states $\mathbf{u}_A$ and $\mathbf{u}_B$ as in $\Delta\varepsilon \coloneqq \mathbf{u}_A - \mathbf{u}_B$, we introduce the operator in above equation which gives:

$$\Delta\varepsilon(t) = \sum\nolimits_i \Delta\varepsilon_{i_0} \exp(\sigma_i t) \mathbf{v}_i \tag{2.22}$$

However, many dynamical systems are either time-dependent or only known over a finite interval of time, which often limits the usability of classical Lyapunov exponent. As a result, we have to resort to advanced concepts like finite-time Lyapunov exponent which we have discussed in section (3.3)

Another way to demonstrate the instability of the system with positive Lyapunov exponents is the *deterministic time horizon* which gives us the duration after which the initial disturbance in direction has grown by the factor ε. Mathematically this is represented as,

$$\tau_{d_i} = \frac{1}{\sigma_i}, \sigma_i > 0 \tag{2.23}$$

Two-Dimensional System

For higher order polynomials, we can write coefficients of the characteristic polynomials in terms of matrix determinants with entries $\operatorname{tr} \mathbf{a}^k$ For two-dimensional systems $\dim(a) = 2$, we can write (2.18) as:

$$\det[\mathbf{a} - \sigma \mathbb{I}] = \sigma^2 - [\operatorname{tr} \mathbf{a}]\sigma + \det \mathbf{a} = 0 \tag{2.24}$$

where the trace and determinant are, respectively

$$\operatorname{tr} \mathbf{a} = a_{11} + a_{22} \tag{2.25}$$

$$\det \mathbf{a} = a_{11}a_{22} - a_{12}a_{21} \tag{2.26}$$

Solving the system gives us the eigenvalues as:

$$\sigma^{\pm} = \frac{1}{2}\operatorname{tr}\mathbf{a} \pm \sqrt{[\operatorname{tr}\mathbf{a}^2] - 4\det\mathbf{a}} \tag{2.27}$$

Hence, we can define the stability of the fixpoint based on following conditions:

1. When $\operatorname{tr}\mathbf{a} < 0$ and $\det\mathbf{a} : \Re(\sigma) < 0$, the fixpoint is stable. When $4\det\mathbf{a} < [\operatorname{tr}\mathbf{a}^2]$, we have two real solutions, therefore perturbations die monotonically. When $4\det\mathbf{a} > [\operatorname{tr}\mathbf{a}^2], \Im(\sigma) \neq 0$,the evolution of the state has an oscillating part. Since , the perturbed state would slowly spiral into fix point.

2. When $\operatorname{tr}\mathbf{a} > 0$ and $\det\mathbf{a} : \Re(\sigma) < 0$, the fixpoint is unstable. Any perturbation would have an exponential growth either in a spiral out or monotonic manner, which would depend on the size of $4\det\mathbf{a}$ and $[\operatorname{tr}\mathbf{a}^2]$.

3. When $\det\mathbf{a} < 0 : \sigma^+$ and σ^-, we get a saddle point as fixpoint, which decays monotonically along ε^-, and grows monotonically along ε^+, the eigenvector with σ^+.

To classify any system into any of the above categories, we need to follow three-steps of calculations. First, we set $\dot{\mathbf{u}} = 0$ and calculate the fixpoint $\mathbf{u}_0$ of the development equation. After this, we calculate the Jacobian matrix $\frac{\delta f_i}{\delta u_j}$ and evaluate it at the fixpoint $\mathbf{u}_0$ to obtain $\mathbf{a}$. And in the last step, we examine $\operatorname{tr}\mathbf{a}$ and $\det\mathbf{a}$, and check their sign $\lesseqgtr 0$ to assign them into aforementioned categories of stability. To have a better understanding, let's look at an example:

Example: Lotka-Voltera Equation for Predator-Prey Systems : This is one of the most famous models in dynamical systems. Let x denote the population of preys such as rabbits and y denote the population of predators such as foxes. Thus, Lotka-Voltera model explains the population dynamics as:

$$\frac{dx}{dt} = ax - bxy \tag{2.28}$$

$$\frac{dy}{dt} = -cy + dxy \tag{2.29}$$

Here, a is the net growth rate of preys in the absence of predators, b is the rate of predation which affects the prey population, c is the death of predators in the absence of prey, and d is the growth rate of predators which is proportionate to food intake.

1. To calculate the fixpoints of the above model, we set $\dot{\mathbf{u}} = f(\mathbf{u})$ where $\mathbf{u} = (x, y)$ This leads to the following:

$$\begin{cases} ax - bxy = 0 \\ -cy + dxy = 0 \end{cases} \implies u_1 = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \text{ and } u_2 = \begin{pmatrix} \frac{c}{d} \\ \frac{a}{b} \end{pmatrix} \tag{2.30}$$

2. Now, we need to calculate the Jacobian matrix

$$\mathbf{a} = \begin{bmatrix} a - by & -bx \\ dy & -c + dx \end{bmatrix} \tag{2.31}$$

We can now calculate trace and determinant at the fixpoints for the above matrix

$$\begin{aligned} \mathbf{a}|_{u=u_1} &= \begin{bmatrix} a & 0 \\ 0 & -c \end{bmatrix} \implies (a-\sigma)(c+\sigma) = 0 \implies \begin{cases} \sigma_1 = a \\ \sigma_2 = -c \end{cases} \\ \mathbf{a}|_{u=u_2} &= \begin{bmatrix} a & -\frac{bc}{d} \\ \frac{ad}{b} & 0 \end{bmatrix} \implies \sigma^2 + ac = 0 \implies \begin{cases} \sigma_1 = -\iota\sqrt{ac} \\ \sigma_2 = \iota\sqrt{ac} \end{cases} \end{aligned} \tag{2.32}$$

3. Thus, $\operatorname{tr}\mathbf{a}|_{u=u_1} = a - c$ and $\det \mathbf{a}|_{u=u_1} = -ac < 0, \sigma_1 > 0, \sigma_2 < 0$, thus u_1 is a saddle point. On the other hand, $\operatorname{tr}\mathbf{a}|_{u=u_2} = 0$ and $\det \mathbf{a}|_{u=u_1} = ac > 0, \Im(\sigma) \neq 0$, thus u_2 is oscillatory.

2.6 Invariant Sets and Manifolds

Invariant sets as the name suggests, is a set of points which is invariant under the development of a dynamical system. The set of fixpoints $\mathbf{u}_0$, where $f(\mathbf{u}_0)$ is one of the simplest examples of such sets. We define the *propagator* $\mathbf{F}_t$ as an operator which maps any state $\mathbf{u}_0$ along the trajectory after time

t. Propagator here macroscopically can be identified as the development operator $\mathfrak{D}$. Mathematically, it's represented as:

$$\mathbf{F}_t(\mathbf{u}(0)) \coloneqq \mathbf{u}(0) + \int_0^t \mathbf{f}(\mathbf{u}(\tau))\,\mathrm{d}\tau = \mathbf{u}(t) \tag{2.33}$$

A set $\mathfrak{S} \subset \mathbb{R}^n$ is an invariant set when for each $\mathbf{u} \in \mathfrak{S}$, the solution $t \mapsto \mathbf{F}_t(\mathbf{u})$ has its image in $\mathfrak{S}$, defined on its maximal interval of existence. If $\mathbf{f}$ is Lipschitz-continuous, and the set is continuous and locally Euclidean, then the manifold is called an *invariant manifold*. A manifold, in general is a topological space that locally resembles Euclidean space near each point.

The manifold can be broadly classified as the *stable, unstable or center manifolds*. Here, we focus on the manifold associated with some fixpoint $\mathbf{u}_0$ and classify the manifolds according to the properties of the fixpoint. We first look at the Jacobian matrix $\mathbf{a}|_{u_0}$ in its eigensystem – with eigenvectors $\mathbf{v}_i$ and the respective eigenvalues σ_i, which characterises into three linear subspaces: (i) *stable subspace* with negative eigenvalues $\sigma < 0$, (ii) *unstable subspace* with $\sigma > 0$, and (iii) *center subspace* with $\sigma = 0$. The tangents to the above subspaces provides us with respective manifolds in each category.

Stable and Unstable Manifolds: In a stable manifold, trajectories approach a fixpoint $\mathbf{u}_0$ exponentially. All the eigenvalues are negative at this point. On the other hand, in an unstable manifold, trajectories get exponentially repelled at the fixpoint. And at such a point, all the eigenvalues are positive here. When there's a mix of both positive and negative eigenvalues at the fixpoint, we get a *hyperbolic saddle point*. Let's look at an example to have a better understanding of such saddle points. Consider a system of differential equations with variables u_1 and u_2, such that:

$$\begin{aligned} \dot{u_1} &= u_1 - \alpha u_2 \\ \dot{u_2} &= \alpha u_1 - u_2 \end{aligned} \tag{2.34}$$

Such equations have a single fixpoint at $(0, 0)$ with eigenvectors $\mathbf{v} = \left(\frac{1}{\alpha}[1 \pm \mu], 1\right)^T$ where $\mu = \sqrt{1 - \alpha^2}$, and corresponding eigenvalues $\pm\mu$.

Center Manifold: When at least one of the eigenvalues of $\mathbf{a}|_{\mathbf{u}_0}$ vanishes, we get a center manifold, whose character is hard to judge from just linear analysis and the dynamics is much slower than exponential.

2.6.1 Invariants manifolds in non-autonomous dynamical systems

A differential equation

$$\dot{\mathbf{u}} = f(\mathbf{u}) \tag{2.35}$$

where $\mathbf{u} \in \mathbb{R}_n, t \in \mathbb{R}$ represents a non-autonomous dynamical system, whose solutions are of the form $\mathbf{u}(t; t_0, \mathbf{u}_0) = f_{t_0}^t(\mathbf{u}_0)$ with $\mathbf{u}(t_0; t_0, \mathbf{u}_0) = \mathbf{u}_0$ represents a non-autonomous dynamical system. In the extended phase space $\mathbb{R}^n \times \mathbb{R}$ of such a system, an invariant manifold is generated by any initial surface $\mathfrak{M}_0 \subset \mathbb{R}^n$

$$\mathfrak{M} = \bigcup_{t \in \mathbb{R}} f_{t_0}^t(\mathfrak{M}_0) \tag{2.36}$$

One really important question is left to be answered, that how can we find such manifolds out of these large families of manifolds, which exert the maximum influence on the overall system dynamics. Such manifolds in the extended phase space for a non-autonomous dynamical systems are known as *Lagrangian Coherent Structures (LCS).*

Chapter 3

Lagrangian Coherent Structures

3.1 Introduction

Material coherence can be observed in the fluid flows all around the globe. Such a coherence emerges as a distinct signature as shown in fig(). *Lagrangian Coherent Strucutres* aim to explain the main cause of such special behaviour observed in fluid flows. LCS acronym was termed by Haller & Yuan(2000) to describe the skeletons of Lagrangian particle dynamics which form the most attracting, repelling and shearing material surfaces. LCS are distinguished separatices in dynamical systems, similar to stable and unstable manifolds of time-independent systems. These invariant manifolds divide dynamically distinct regions in the flow and enforce a major influence on nearby trajectories over time. The kind of this influence may vary, but it invariably creates a coherent surface for which the underlying LCS serves as a skeleton.

Attracting LCS are the separatices which attracts the nearby trajectories over the time $[t_0, t]$ with the maximum intensity for the times $\tau \in [t_0, t]$. Therefore, the attracting LCS are responsible for making the centrepiece where the nearby trajectories compile for the forward-evolving trajectory patterns over the time interval $[t_0, t]$. Per se, in unsteady flows these LCS make the theoretical centrepieces of tracer filaments.

Accordingly, repelling LCS are the separatices which repel the nearby trajectories over the $[t_0, t]$ with the maximum intensity for times $\tau \in [t_0, t]$. Such strong repulsive elements cause the nearby trajectories to diverge and propagate to different areas in domain. In particular, repelling LCSs serve as the theoretical centrepieces of major local stretching regions as seen in the unsteady flows. In backward time, repelling LCSs become attracting LCSs and vice versa.

LCS examples seen in real world includes oil spills, floating debris, chlorophyll patterns in the ocean, spores in the atmosphere.

3.2 General Definitions

3.2.1 Material Surfaces

Consider a non-autonomous dynamical system defined by a development operator or flow map $f_{t_0}^t : \mathbf{u}_0 \mapsto \mathbf{u}(t; t_0, \mathbf{u}_0)$ on a phase space $\mathfrak{P}$ and over a time interval $\mathfrak{I} = [t_0, t_1]$. The development operator maps any initial condition $\mathbf{u}_0 \in \mathfrak{P}$ for any time $t \in \mathfrak{I}$ to a final condition $\mathbf{u}(t, t_0, \mathbf{u}_0) \in \mathfrak{P}$. If the function $f_{t_0}^t$ is diffeomorphic i.e. the function and it's inverse are smooth, then the set

$$\mathfrak{M} = (\mathbf{u}, t) \in \mathfrak{P} \times \mathfrak{I} : [f_{t_0}^t]^{-1}(\mathbf{u}) \in \mathfrak{M}(t_0) \tag{3.1}$$

is an *invariant manifold* in the extended phase space $\mathfrak{P} \times \mathfrak{I}$, where $\mathfrak{M}(t_0)$ is any smooth set of initial conditions in $\mathfrak{P}$. Such an evolving time slice $\mathfrak{M}(t) = f_{t_0}^t(\mathfrak{M}(t_0))$ is known as *material surfaces* in fluid dynamics.

3.2.2 Exceptional Material Surfaces

Any material surface $\mathfrak{M}(t)$ should employ a stable and consistent action on nearby trajectories to form a coherent pattern over time interval $\mathfrak{I}$. Depending on the kind of property such actions exert, they can be classified into attraction, repulsion or shear. We have already discussed in section 2.4.1 about these properties for classical dynamical systems and the inequalities associated with them. Henceforth, from there we can conclude that for any material surface $\mathfrak{M}(t)$, if in a flow a small initial perturbation to $\mathfrak{M}(t_0)$ results into even smaller perturbations $\mathfrak{M}(t_1)$, then such a surface is attracting, where if in a flow a small initial perturbation to $\mathfrak{M}(t_0)$ results into bigger perturbations $\mathfrak{M}(t_1)$, then such a surface is repelling.

Now, let's focus on a more complex case and consider a dynamical system over a finite time interval $\mathfrak{I}$. Such strict inequalities that we have seen before don't necessarily define locally unique material surface. The reason for this is the continuity of the development operator $f_{t_0}^t$ over $\mathfrak{I}$, which makes any surface close to attracting material surface $\mathfrak{M}(t)$ is also attracting the nearby trajectories. This results in stacking of the different attracting, repelling and shearing material surfaces on each other. The surface amongst these family of surfaces which exhibits the strongest coherence property is the main idea behind coining LCSs. Such extremas serve as the centerpiece in the trajectory patterns, as shown in

3.2.3 Hyperbolic LCSs

The above definitions thus makes it possible to define the *attracting LCSs* and *repelling LCSs* in the extended phase space $\mathfrak{P} \times \mathfrak{I}$. Together, the attracting and repelling LCSs are called *hyperbolic LCSs.*

Let's consider a hyperbolic point which has an attracting and a repelling manifold as shown in fig(). If we consider two points on either side of an attracting manifold and develop them in time, we will find that they diverge from each other. Similarly, if we start these points from either side of repelling manifold and develop backward in time, the points will converge. That's why such surfaces are called *separatices* because they separate the region with different qualitative dynamics. The stretching between the trajectories in these regions can in turn help us to define such separatices or LCSs. We measure the stretching forward in time when considering separatices similar to attracting manifolds and backward in time for separatices similar to repelling manifolds. To physically measure the stretching, we use *Finite-Time Lyapunov Exponent.*

3.3 The Finite-Time Lyapunov Exponent

The finite-time Lyapunov exponent (FTLE), represented by $\sigma_t^T(\mathbf{u})$, is a scalar value which characterises the amount of stretching of point $\mathbf{u} \in \mathfrak{M}$ about the trajectory over the time interval $[t, t+T]$. FTLE is a function of both time and space. The FTLE represents an average, integrated effect between trajectories, and shouldn't be confused as an instantaneous separation measure.

3.3.1 FLow Map

Let's now formulate an FTLE expression and consider stretching between two neighboring particles in a flow. Let's consider a point $\mathbf{u} \in \mathfrak{M}$ at time t_0

and a development operator or flow map $f_{t_0}^{t_0+T}$ which maps any point to a future state at time $t_0 + T$ such that:

$$\mathbf{u} \mapsto f_{t_0}^{t_0+T}(\mathbf{u}) \tag{3.2}$$

The neighbouring point of $\mathbf{u}$ at t_0 will behave similarly to $\mathbf{u}$ locally, as the flow is continually dependent on the initial conditions. As time progresses, the distance between the two points will most certainly change. Let's represent the neighbouring particle as $\mathbf{v} = \mathbf{u} + \delta\mathbf{u}(t_0)$, where $\delta\mathbf{u}(t_0)$ is the infinitesimal distance between these particles. On doing a Taylor expansion around $\mathbf{u}$, the perturbation evolves with advection time T as following:

$$\delta\mathbf{u}(t_0 + T) = f_{t_0}^{t_0+T}(\mathbf{v}) - f_{t_0}^{t_0+T}(\mathbf{u}) = \frac{\mathrm{d}f_{t_0}^{t_0+T}(\mathbf{u})}{\mathrm{d}\mathbf{u}}\delta(\mathbf{u}(t_0)) + \mathcal{O}(\| \delta\mathbf{u}(t_0) \|)^2 \tag{3.3}$$

3.3.2 Strain Tensors

In order to understand Lagrangian coherence, we need to explore material surfaces $\mathfrak{M}(t)$ which have an exceptional impact on the deformation of nearby material elements.The development of infinitesimal perturbations $\delta\mathbf{u}(t_0)$ to the trajectory is a reflection of local deformation in the trajectories. In (3.3) it's safe to ignore $\mathcal{O}(\| \delta\mathbf{u}(t_0) \|)^2$ since $\delta(\mathbf{u}(t_0)$ is assumed to be infinitesimal. The magnitude of perturbation can be found by taking the L_2 norm of (3.3),

$$\begin{aligned} \| \delta(\mathbf{u}(t_0)) \| &= \sqrt{\left\langle \frac{\mathrm{d}f_{t_0}^{t_0+T}(\mathbf{u})}{\mathrm{d}\mathbf{u}}\delta(\mathbf{u}(t_0)), \frac{\mathrm{d}f_{t_0}^{t_0+T}(\mathbf{u})}{\mathrm{d}\mathbf{u}}\delta(\mathbf{u}(t_0)) \right\rangle} \\ &= \sqrt{\left\langle \delta(\mathbf{u}(t_0)), \frac{\mathrm{d}f_{t_0}^{t_0+T}(\mathbf{u})}{\mathrm{d}\mathbf{u}}^T \frac{\mathrm{d}f_{t_0}^{t_0+T}(\mathbf{u})}{\mathrm{d}\mathbf{u}}\delta(\mathbf{u}(t_0)) \right\rangle} \end{aligned} \tag{3.4}$$

where the notation M^T denotes the transpose matrix of M. The symmetric matrix

$$\Delta = \frac{\mathrm{d}f_{t_0}^{t_0+T}(\mathbf{u})}{\mathrm{d}\mathbf{u}}^T \frac{\mathrm{d}f_{t_0}^{t_0+T}(\mathbf{u})}{\mathrm{d}\mathbf{u}} \tag{3.5}$$

is a finite-time version of Cauchy-Green strain tensor. The symmetric tensor is positive definite as $\nabla f_{t_0}^{t_0+T}$ is invertible. Thus, the eigenvalues $\lambda_i(\mathbf{u}_0)$ and eigenvectors $\xi_i(\mathbf{u}_0)$ of matrix Δ satisfy

$$\begin{aligned} \Delta\xi_i = \lambda_i(\mathbf{u}_0), \quad |\xi_i| = 1, \quad i = 1, \ldots, n; \\ \text{s.t.} \quad 0 < \lambda_1 \leq \cdots \leq \lambda_n, \quad \xi_i \perp \xi_j, \quad i \neq j, \end{aligned} \tag{3.6}$$

where $n = 2$ for two-dimensional flows and $n = 3$ for three-dimensional flows.

3.3.3 Computing the Deformation Gradient

The flow map and it's gradient aren't objective functions. Solving (3.3) will give noisy results for $\nabla f_{t_0}^{t_0+T}(\mathbf{u}_0)$ as a function of $\mathbf{u}_0$. Instead, for Lagrangian coherence calculations, Haller suggested the following finite-difference approximation for a two-dimensional flow

$$\nabla f_{t_0}^{t_0+T} \approx \begin{pmatrix} \frac{\mathbf{u}^1(t;t_0,\mathbf{u}_0+\delta_1)-\mathbf{u}^1(t;t_0,\mathbf{u}_0-\delta_1)}{|2\delta_1|} & \frac{\mathbf{u}^1(t;t_0,\mathbf{u}_0+\delta_2)-\mathbf{u}^1(t;t_0,\mathbf{u}_0-\delta_2)}{|2\delta_2|} \\ \frac{\mathbf{u}^2(t;t_0,\mathbf{u}_0+\delta_1)-\mathbf{u}^2(t;t_0,\mathbf{u}_0-\delta_1)}{|2\delta_1|} & \frac{\mathbf{u}^2(t;t_0,\mathbf{u}_0+\delta_2)-\mathbf{u}^2(t;t_0,\mathbf{u}_0-\delta_2)}{|2\delta_2|} \end{pmatrix} \tag{3.7}$$

with a small vector δ_i pointing in the $\mathbf{u}^i$ coordinate direction. Often, higher dimensions are subjected to two-dimensional approximations to save computational costs.

3.3.4 Deriving FTLE

Following our earlier derivations, let's again focus on the two neighbouring particles $\mathbf{u}$ and $\mathbf{v}$. We wish to calculate the maximum stretching that occurs between these two points and naturally, this will happen when $\delta\mathbf{u}(t_0)$ is chosen such that it aligns with the eigenvector associated with the maximum eigenvalue of Δ. Therefore, if we assume the maximum eigenvalue of Δ to be $\lambda_{\max}(\Delta)$, we get

$$\begin{aligned} \max_{\delta\mathbf{u}(t_0)} \parallel \delta\mathbf{u}(t_0+T) \parallel &= \sqrt{\langle \overline{\delta\mathbf{u}}(t_0), \lambda_{\max}(\Delta)\overline{\delta\mathbf{u}}(t_0) \rangle} \\ &= \sqrt{\lambda_{\max}(\Delta)} \parallel \overline{\delta\mathbf{u}}(t_0) \parallel, \end{aligned} \tag{3.8}$$

where $\overline{\delta\mathbf{u}}(t_0)$ is aligned with the eigenvector associated with $\lambda_{\max}(\Delta)$. Now, if we define the finite-time Lyapunov Exponent as:

$$\sigma_{t_0}^{T}(\mathbf{u}) = \frac{1}{|T|} \ln \sqrt{\lambda_{\max}(\Delta)}, \tag{3.9}$$

then, the average exponent of growth can be determined from (3.8):

$$\max_{\delta\mathbf{u}(t_0)} \parallel \delta\mathbf{u}(t_0 + T) \parallel = \mathrm{e}^{\sigma_{t_0}^{T}(\mathbf{u})|T|} \parallel \overline{\delta\mathbf{u}}(t_0) \parallel \tag{3.10}$$

The Eq.(3.10) gives us the finite-time Lyapunov exponent at point $\mathbf{u} \in \mathfrak{M}$ at time t_0 with integration time T.

3.4 LCS as FTLE Ridges

3.4.1 What is a Ridge?

Before jumping straight to LCS detection, let's first define a *ridge*. Physically, a ridge or a mountain ridge is a geological feature that is formed for some distance by a chain of mountains or hills as a continuous elevated crest. The line formed by connecting the highest points along the crest, with terrain dropping on either side is called a *ridgeline*.

Mathematically for a smooth function with two variables, the ridges are a set of curves whose points are a local maxima of the function in atleast one dimension. Extending this definition for a function with N variables, the ridges are a set of curves whose points are local maxima in *N - 1* dimensions. Au contraire, if we consider the set of curves with local minima, analogously we get *valleys*. The union of ridge sets and valley sets, along with a related set of point s known as *connector set* collectively form a connected set of curves that meet, partition or intersect at the critical points of the function. Such a union is known as function's *relative critical set*.

3.4.2 Ridge in N dimensions

General Defintion: Consider a function $f : \mathbb{R}^n \to \mathbb{R}$, where a point $\mathbf{u}_0$ exists in the domain such that for any point $\mathbf{u}$ in the neighbourhood of $\mathbf{u}_0$, the condition $f(u) < f(u_0)$ holds, then $\mathbf{u}_0$ is a *local maxima* of the function. When this condition holds for the entire domain, then $\mathbf{u}_0$ is the *global maxima*.

If we slightly relax the condition $f(u) < f(u_0)$ for $\mathbf{u}$ in the entire neighbourhood of $\mathbf{u}_0$ such that it holds on an *n-1* dimensional subset, it allows the set of maximal points to have a single degree of freedom. This will lead to the sets of points forming a $1 - D$ locus, or a ridge curve.

Eberly's Definition: Another more sophisticated definition of rigdes was coined by Eberly. Let $\mathfrak{S} \subset \mathbb{R}^n$ be an open set, and $f : \mathfrak{S} \to \mathbb{R}$ be smooth. Let $\mathbf{u}_0 \in \mathfrak{S}$, and $\nabla_{\mathbf{u}_0} f$ be the gradient at $\mathbf{u}_0$, and $H_{\mathbf{u}_0}(f)$ be the $n \times n$ Hessian matrix of f at $\mathbf{u}_0$. Let $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ be the n ordered eigenvalues of $H_{\mathbf{u}_0}$, and let $\mathbf{e}_i$ be a unit eigenvector in the eigenspace for λ_i, then the point $\mathbf{u}_0$ is on the $1 - D$ ridge if the following conditions hold true:

1. $\lambda_{n-1} < 0$, and

2. $\nabla_{\mathbf{u}_0} f \cdot \mathbf{e}_i = 0$ for $i = 1, 2, \ldots, n-1$

Extending this definition for a k-dimensional ridge, if following conditions hold:

1. $\lambda_{n-k} < 0$, and

2. $\nabla_{\mathbf{u}_0} f \cdot \mathbf{e}_i = 0$ for $i = 1, 2, \ldots, n-k$

then, $\mathbf{u}_0$ is a point on k-dimensional ridge of f.

3.4.3 Pseudo code for 2D Ridge Extraction

For this thesis, we developed a 2-dimensional ridge extraction software. Here is a short pseudo code of the method used:

```
Algorithm 1 Ridgeline Extraction
Data: Node based Scalar Data
Result: RidgeLine Extraction
begin;
 while $\boldsymbol{u} = (x, y) \in \mathfrak{M}$, at each node: do
     • Gradient $\nabla_{\mathbf{u}}$ calculation
     • Hessian $H_{\mathbf{u}}$ calculation
     • Eigenvalues $\sigma_i$ and eigenvectors $\lambda_i$ calculation
         – get: Min eigenvalue $\sigma_{i_{\min}}$ and corresponding eigenvector $\lambda_{i_{\min}}$
end
while $\boldsymbol{u} = (x, y) \in \mathfrak{M}$, at each cell: do
     • Principal Component Analysis.
         – get: Max eigenvector $\lambda_{p_{\max}}$
     • Dot product between $\lambda_{i_{\min}}$ and $\lambda_{p_{\max}}$
         – if Dot Product < 0 then
               flip the direction of $\lambda_{i_{\min}}$
           end
     • Mark every node as + or - by isolines, depending on the isoline conditions $f_i \geq c, f_i < c$, where $f = \nabla_{\mathbf{u}_i} \cdot \lambda_{i_{\min}}$
     • Use look up table to identify respective cases of marked nodes
     • Find exact position of intersection on edge using linear interpolation
     • Interpolate hessian $H_{\mathbf{u}_0}$ to the intersection point for all points
         – Calculate eigenvalues $\sigma_j$
             * if $\vee$ any i, $\sigma_i$ < user input limit then
                   Store the point
               else
                   Discard
               end
end
```

3.4.4 FTLE Ridges

Locating LCSs usually involves a wide study of stability of material surfaces in flow domain. One approach could be to search for the material surfaces along which the infinitesimal deformation is largest or smallest. Haller () proposed that at time t_0, an attracting LCS over $[t_0, t_0+T]$ is a a maximizing curve, or ridge of the backward-time FTLE field, whereas on the other hand a repelling LCS over $[t_0, t_0 + T]$ should be the ridge of forward time FTLE. Let's look at an example to better understand how FTLE is used to detect LCS:

Example 3.4.1. ***Time-Independent Double Gyre***

Let's consider a simple example of stream function given by following equation:

$$\psi(x, y) = \sin(\pi x) \sin(\pi y) \tag{3.11}$$

over the region $\mathfrak{M} = [0, 2] \times [0, 1]$. *By definition, the velocity field is:*

$$\begin{aligned} \dot{x} &= -\frac{\mathrm{d}\psi}{\mathrm{d}y} = -\pi \sin(\pi x) \cos(\pi y) \\ \dot{y} &= \frac{\mathrm{d}\psi}{\mathrm{d}x} = \pi \cos(\pi x) \sin(\pi y) \end{aligned} \tag{3.12}$$

The velocity field and streamlines for the above set of equations look like following:

If we look closely at the image, we find various *heteroclinic trajectories.* Heteroclinic trajectories separate distinct regions of the flow, that's why can also be considered as separatices. One such separatix which is most apparently visible is between the fixed points at $(1, 0)\text{and}(1, 1)$. Also, the trajectories at the boundaries are also separatices. Let's consider three points near the separatrix as shown in the image below and notice how the streamline evolves with time. We notice that the points $A\text{and}B$ remain closer, but the the point C diverges from the other particles with time. Thus, intuitively with the definitions so far, we can assume that the FTLE values should be large around this separatrix.

If we compute the FTLE, we find out infact a relatively higher value of FTLE at all the separatices as can be seen in the images below. Such ridges of high FTLE are infact known as LCSs.

3.4.5 Pseudo code for Time-Dependent FTLE

```
Algorithm 2 Time-dependent FTLE
Data: Node based time-dependent velocity data
Input: Start time $t_0$, Advection time $\tau$
Result: FTLE, Pathlines
begin;
  Store: All time stamps as Multiblock data set
  if $\tau > 0$ then
    Forward FTLE
else
    Backward FTLE: Reverse the velocity fields
end
Pathline:
  for $i \leftarrow t_0$ to $t_0 + \tau$ by $i =$ next time step do
      • Get two consecutive time stamps of velocity fields
      • for $\boldsymbol{u} = (x, y) \in \mathfrak{M}$ do
            – Interpolate velocity between two velocity fields as time progresses.
            – Integrate till it reaches the next time stamp
            – Store the endpoint of pathline
        end
      • Use the end points from last iteration as start points for next iteration.
end
FTLE:
  Get: Endpoints of the pathline after final iteration
  for every $\boldsymbol{u}_{end} = (x_{end}, y_{end}) \in \mathfrak{M}$ do
      • Jacobian $\mathbf{J}$, $\mathbf{J}^T$ and multiply both matrices
      • Calculate eigenvalues and find the maximum eigenvalue $\lambda_{\max}$
      • Calculate $\frac{1}{\tau} \ln \sqrt{\lambda_{\max}}$ to get FTLE
end
```