TURBULENCE, ENTROPY
AND DYNAMICS

Lecture Notes, UPC 2014

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Chapter 1

Turbulence

For other uses, see Turbulence (disambiguation).

In fluid dynamics, turbulence or turbulent flow is a flow regime characterized by chaotic property changes. This includes low momentum diffusion, high momentum convection, and rapid variation of pressure and velocity in space and time.

Flow in which the kinetic energy dies out due to the action of fluid molecular viscosity is called laminar flow. While there is no theorem relating the non-dimensional Reynolds number (Re) to turbulence, flows at Reynolds numbers larger than 5000 are typically (but not necessarily) turbulent, while those at low Reynolds numbers usually remain laminar. In Poiseuille flow, for example, turbulence can first be sustained if the Reynolds number is larger than a critical value of about 2040;[1] moreover, the turbulence is generally interspersed with laminar flow until a larger Reynolds number of about 4000.

In turbulent flow, unsteady vortices appear on many scales and interact with each other. Drag due to boundary layer skin friction increases. The structure and location of boundary layer separation often changes, sometimes resulting in a reduction of overall drag. Although laminar-turbulent transition is not governed by Reynolds number, the same transition occurs if the size of the object is gradually increased, or the viscosity of the fluid is decreased, or if the density of the fluid is increased. Nobel Laure-
ate Richard Feynman described turbulence as “the most important unsolved problem of classical physics.”[2]

1.1 Features

Turbulence is characterized by the following features:

- Irregularity: Turbulent flows are always highly irregular. For this reason, turbulence problems are normally treated statistically rather than deterministically. Turbulent flow is chaotic. However, not all chaotic flows are turbulent.

- Diffusivity: The readily available supply of energy in turbulent flows tends to accelerate the homogenization (mixing) of fluid mixtures. The characteristic which is responsible for the enhanced mixing and increased rates of mass, momentum and energy transports in a flow is called “diffusivity”.

- Rotationality: Turbulent flows have non-zero vorticity and are characterized by a strong three-dimensional vortex generation mechanism known as vortex stretching. In fluid dynamics, they are essentially vortices subjected to stretching associated with a corresponding increase of the component of vorticity in the stretching direction—due to the conservation of angular momentum. On the other hand, vortex stretching is the core mechanism on which the turbulence energy cascade relies to establish the structure function. In general, the stretching mechanism implies thinning of the vortices in the direction perpendicular to the stretching direction due to volume conservation of fluid elements. As a result, the radial length scale of the vortices decreases and the larger flow structures break down into smaller structures. The process continues until the small scale structures are small enough that their kinetic energy can be transformed by the fluid’s molecular viscosity into heat. This is why turbulence is always rotational and three dimensional. For example, atmospheric cyclones are rotational but their substantially two-dimensional shapes do not allow vortex generation and so are not turbulent. On the other hand, oceanic flows are dispersive but essentially non rotational and therefore are not turbulent.

- Dissipation: To sustain turbulent flow, a persistent source of energy supply is required because turbulence dissipates rapidly as the kinetic energy is converted into internal energy by viscous shear stress.

Turbulent diffusion is usually described by a turbulent diffusion coefficient. This turbulent diffusion coefficient is defined in a phenomenological sense, by analogy with the molecular diffusivities, but it does not have a true physical meaning, being dependent on the flow conditions, and not a property of the fluid itself. In addition, the turbulent diffusivity concept assumes a constitutive relation between a turbulent flux and the gradient of a mean variable similar to the relation between flux and gradient that exists for molecular transport. In the best case, this assumption is only an approximation. Nevertheless, the turbulent diffusivity is the simplest approach for quantitative analysis of turbulent flows, and many models have been postulated to calculate it. For instance, in large bodies of water like oceans this coefficient can be found using Richardson’s four-third power law and is governed by the random walk principle. In rivers and large ocean currents, the diffusion coefficient is given by variations of Elder’s formula.

Turbulence causes the formation of eddies of many different length scales. Most of the kinetic energy of the turbulent motion is contained in the large-scale structures. The energy “cascades” from these large-scale structures to smaller scale structures by an inertial and essentially inviscid mechanism. This process continues, creating smaller and smaller structures which produces a hierarchy of eddies. Eventually this process creates structures that are small enough that molecular diffusion becomes important and viscous dissipation of energy finally takes place. The scale at which this happens is the Kolmogorov length scale.

Via this energy cascade, turbulent flow can be realized as a superposition of a spectrum of velocity fluctuations and eddies upon a mean flow. The eddies are loosely defined as coherent patterns of velocity, vorticity and pressure. Turbulent flows may be viewed as made of an entire hierarchy of eddies over a wide range of length scales and the hierarchy can be described by the energy spectrum that measures the energy in velocity fluctuations for each length scale (wavenumber). The scales in the energy cascade are generally uncontrollable and highly non-symmetric. Nevertheless, based on these length scales these eddies can be divided into three categories.

1. Integral length scales: Largest scales in the energy spectrum. These eddies obtain energy from the mean flow and also from each other. Thus, these are the energy production eddies which contain most of the energy. They have the large velocity fluctuation and are low in frequency. Integral scales are highly anisotropic and are defined in terms of the normalized two-point velocity correlations. The maximum length of these scales is constrained by the characteristic length of the apparatus. For example, the largest integral length scale of pipe flow is equal to the pipe diameter. In the case of atmospheric turbulence, this length can reach up to the order of several hundreds kilometers.

2. Kolmogorov length scales: Smallest scales in the spectrum that form the viscous sub-layer range. In this range, the energy input from nonlinear interactions and the energy drain from viscous dissipation are in exact balance. The small scales have high
frequency, causing turbulence to be locally isotropic and homogeneous.

3. Taylor microscales: The intermediate scales between the largest and the smallest scales which make the inertial subrange. Taylor micro-scales are not dissipative scale but pass down the energy from the largest to the smallest without dissipation. Some literatures do not consider Taylor micro-scales as a characteristic length scale and consider the energy cascade to contain only the largest and smallest scales; while the latter accommodate both the inertial sub-range and the viscous-sub layer. Nevertheless, Taylor micro-scales are often used in describing the term “turbulence” more conveniently as these Taylor micro-scales play a dominant role in energy and momentum transfer in the wavenumber space.

Although it is possible to find some particular solutions of the Navier-Stokes equations governing fluid motion, all such solutions are unstable to finite perturbations at large Reynolds numbers. Sensitive dependence on the initial and boundary conditions makes fluid flow irregular both in time and in space so that a statistical description is needed. The Russian mathematician Andrey Kolmogorov proposed the first statistical theory of turbulence, based on the aforementioned notion of the energy cascade (an idea originally introduced by Richardson) and the concept of self-similarity. As a result, the Kolmogorov microscales were named after him. It is now known that the self-similarity is broken so the statistical description is presently modified. Still, a complete description of turbulence remains one of the unsolved problems in physics.

According to an apocryphal story, Werner Heisenberg was asked what he would ask God, given the opportunity. His reply was: “When I meet God, I am going to ask him two questions: Why relativity? And why turbulence? I really believe he will have an answer for the first.” A similar witticism has been attributed to Horace Lamb (who had published a noted text book on Hydrodynamics)—his choice being quantum electrodynamics (instead of relativity) and turbulence. Lamb was quoted as saying in a speech to the British Association for the Advancement of Science, “I am an old man now, and when I die and go to heaven there are two matters on which I hope for enlightenment. One is quantum electrodynamics, and the other is the turbulent motion of fluids. And about the former I am rather optimistic.”

A more detailed presentation of turbulence with emphasis on high-Reynolds number flow, intended for a general readership of physicists and applied mathematicians, is found in the Scholarpedia articles by R. Benzi and U. Frisch and by G. Falkovich. There are many scales of meteorological motions; in this context turbulence affects small-scale motions.

1.2 Examples of turbulence

- Smoke rising from a cigarette is turbulent flow. For the first few centimeters, the flow is certainly laminar. Then smoke becomes turbulent as its Reynolds number increases, as its velocity and characteristic length are both increasing.

- Flow over a golf ball. (This can be best understood by considering the golf ball to be stationary, with air flowing over it.) If the golf ball were smooth, the boundary layer flow over the front of the sphere would be laminar at typical conditions. However, the boundary layer would separate early, as the pressure gradient switched from favorable (pressure decreasing in the flow direction) to unfavorable (pressure increasing in the flow direction), creating a large region of low pressure behind the ball that creates high form drag. To prevent this from happening, the surface is dimpled to perturb the boundary layer and promote transition to turbulence. This results in higher skin friction, but moves the point of boundary layer separation further along, resulting in lower form drag and lower overall drag.

- The mixing of warm and cold air in the atmosphere by wind, which causes clear-air turbulence experienced during airplane flight, as well as poor astronomical seeing (the blurring of images seen through the atmosphere.)

- Most of the terrestrial atmospheric circulation

- The oceanic and atmospheric mixed layers and intense oceanic currents.

- The flow conditions in many industrial equipment (such as pipes, ducts, precipitators, gas scrubbers, dynamic scraped surface heat exchangers, etc.) and machines (for instance, internal combustion engines and gas turbines).

- The external flow over all kinds of vehicles such as cars, airplanes, ships and submarines.

- The motions of matter in stellar atmospheres.

- A jet exhausting from a nozzle into a quiescent fluid. As the flow emerges into this external fluid, shear layers originating at the lips of the nozzle are created. These layers separate the fast moving jet from the external fluid, and at a certain critical Reynolds number they become unstable and break down to turbulence.

- Snow fences work by inducing turbulence in the wind, forcing it to drop much of its snow load near the fence.

- Bridge supports (piers) in water. In the late summer and fall, when river flow is slow, water flows
smoothly around the support legs. In the spring, when the flow is faster, a higher Reynolds Number is associated with the flow. The flow may start off laminar but is quickly separated from the leg and becomes turbulent.

- In many geophysical flows (rivers, atmospheric boundary layer), the flow turbulence is dominated by the coherent structure activities and associated turbulent events. A turbulent event is a series of turbulent fluctuations that contain more energy than the average flow turbulence. In his original theory of 1941, Kolmogorov postulated that for very high Reynolds numbers, the small scale turbulent motions are statistically isotropic (i.e. no preferential spatial direction could be discerned). In general, the large scales of a flow are not isotropic, since they are determined by the particular geometrical features of the boundaries (the size characterizing the large scales will be denoted as $L$). Kolmogorov’s idea was that in the Richardson’s energy cascade this geometrical and directional information is lost, while the scale is reduced, so that the statistics of the small scales has a universal character: they are the same for all turbulent flows when the Reynolds number is sufficiently high.

Thus, Kolmogorov introduced a second hypothesis: for very high Reynolds numbers the statistics of small scales are universally and uniquely determined by the viscosity $\nu$ and the rate of energy dissipation (\(\varepsilon\)). With only these two parameters, the unique length that can be formed by dimensional analysis is

$$\eta = \left( \frac{\nu^3 \lambda}{\varepsilon} \right)^{1/4}$$

This is today known as the Kolmogorov length scale (see Kolmogorov microscales).

1.3 Heat and momentum transfer

When flow is turbulent, particles exhibit additional transverse motion which enhances the rate of energy and momentum exchange between them thus increasing the heat transfer and the friction coefficient.

Assume for a two-dimensional turbulent flow that one was able to locate a specific point in the fluid and measure the actual velocity $v = (v_x, v_y)$ of every particle that passed through that point at any given time. Then one would find the actual velocity fluctuating about a mean value:

$$v_x = \overline{v_x} + v'_x$$

and similarly for temperature ($T = \overline{T} + T'$) and pressure ($P = \overline{P} + P'$), where the primed quantities denote fluctuations superposed to the mean. This decomposition of a flow variable into a mean value and a turbulent fluctuation was originally proposed by Osborne Reynolds in 1895, and is considered to be the beginning of the systematic mathematical analysis of turbulent flow, as a sub-field of fluid dynamics. While the mean values are taken as predictable variables determined by dynamics laws, the turbulent fluctuations are regarded as stochastic variables.

The heat flux and momentum transfer (represented by the shear stress $\tau$) in the direction normal to the flow for a given time are

$$q = v'_y \rho c_p T' = -k_{turb} \frac{\partial T}{\partial y}$$

and

$$\tau = -\rho v'_y v'_x = \mu_{turb} \frac{\partial v_x}{\partial y}$$

where $c_p$ is the heat capacity at constant pressure, $\rho$ is the density of the fluid, $\mu_{turb}$ is the coefficient of turbulent viscosity and $k_{turb}$ is the turbulent thermal conductivity.
A turbulent flow is characterized by a hierarchy of scales through which the energy cascade takes place. Dissipation of kinetic energy takes place at scales of the order of Kolmogorov length \( \eta \), while the input of energy into the cascade comes from the decay of the large scales, of order \( L \). These two scales at the extremes of the cascade can differ by several orders of magnitude at high Reynolds numbers. In between there is a range of scales (each one with its own characteristic length \( r \)) that has formed at the expense of the energy of the large ones. These scales are very large compared with the Kolmogorov length, but still very small compared with the large scale of the flow (i.e. \( \eta \ll r \ll L \)). Since eddies in this range are much larger than the dissipative eddies that exist at Kolmogorov scales, kinetic energy is essentially not dissipated in this range, and it is merely transferred to smaller scales until viscous effects become important as the order of the Kolmogorov scale is approached. Within this range inertial effects are still much larger than viscous effects, and it is possible to assume that viscosity does not play a role in their internal dynamics (for this reason this range is called “inertial range”).

Hence, a third hypothesis of Kolmogorov was that at very high Reynolds number the statistics of scales in the range \( \eta \ll r \ll L \) are universally and uniquely determined by the scale \( r \) and the rate of energy dissipation \( \varepsilon \).

The way in which the kinetic energy is distributed over the multiplicity of scales is a fundamental characterization of a turbulent flow. For homogeneous turbulence (i.e., statistically invariant under translations of the reference frame) this is usually done by means of the energy spectrum function \( E(k) \), where \( k \) is the modulus of the wavevector corresponding to some harmonics in a Fourier representation of the flow velocity field \( \mathbf{u}(x) \):

\[
\mathbf{u}(x) = \int \int \int_{\mathbb{R}^3} \hat{\mathbf{u}}(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}}d^3k
\]

where \( \hat{\mathbf{u}}(\mathbf{k}) \) is the Fourier transform of the velocity field. Thus, \( E(k)dk \) represents the contribution to the kinetic energy from all the Fourier modes with \( k < |\mathbf{k}| < k + dk \), and therefore,

\[
\frac{1}{2} \langle u_i u_i \rangle = \int_0^\infty E(k)dk
\]

where \( \frac{1}{2} \langle u_i u_i \rangle \) is the mean turbulent kinetic energy of the flow. The wavenumber \( k \) corresponding to length scale \( r \) is \( k = 2\pi / r \). Therefore, by dimensional analysis, the only possible form for the energy spectrum function according with the third Kolmogorov’s hypothesis is

\[
E(k) = C \varepsilon^{2/3} k^{-5/3}
\]

where \( C \) would be a universal constant. This is one of the most famous results of Kolmogorov 1941 theory, and considerable experimental evidence has accumulated that supports it.\(^{13}\)

In spite of this success, Kolmogorov theory is at present under revision. This theory implicitly assumes that the turbulence is statistically self-similar at different scales. This essentially means that the statistics are scale-invariant in the inertial range. A usual way of studying turbulent velocity fields is by means of velocity increments:

\[
\delta\mathbf{u}(r) = \mathbf{u}(\mathbf{x} + r) - \mathbf{u}(\mathbf{x})
\]

that is, the difference in velocity between points separated by a vector \( r \) (since the turbulence is assumed isotropic, the velocity increment depends only on the modulus of \( r \)). Velocity increments are useful because they emphasize the effects of scales of the order of the separation \( r \) when statistics are computed. The statistical scale-invariance implies that the scaling of velocity increments should occur with a unique scaling exponent \( \beta \), so that when \( r \) is scaled by a factor \( \lambda \),

\[
\delta\mathbf{u}(\lambda r)
\]

should have the same statistical distribution as

\[
\lambda^\beta \delta\mathbf{u}(r)
\]

with \( \beta \) independent of the scale \( r \). From this fact, and other results of Kolmogorov 1941 theory, it follows that the statistical moments of the velocity increments (known as structure functions in turbulence) should scale as

\[
\langle [\delta\mathbf{u}(r)]^n \rangle = C_n \varepsilon^{n/3} r^{n/3}
\]

where the brackets denote the statistical average, and the \( C_n \) would be universal constants.

There is considerable evidence that turbulent flows deviate from this behavior. The scaling exponents deviate from the \( n/3 \) value predicted by the theory, becoming a non-linear function of the order \( n \) of the structure function. The universality of the constants have also been questioned. For low orders the discrepancy with the Kolmogorov \( n/3 \) value is very small, which explain the success of Kolmogorov theory in regards to low order statistical moments. In particular, it can be shown that when the energy spectrum follows a power law

\[
E(k) \propto k^{-p}
\]

with \( 1 < p < 3 \), the second order structure function has also a power law, with the form

\[
\langle [\delta\mathbf{u}(r)]^2 \rangle = C_2 \varepsilon^{5/3} r^{5/3}
\]
\[ \langle [\delta u(r)]^2 \rangle \propto r^{P-1} \]

Since the experimental values obtained for the second order structure function only deviate slightly from the 2/3 value predicted by Kolmogorov theory, the value for \( p \) is very near to 5/3 (differences are about 2\%\(^{[14]} \)). Thus the “Kolmogorov –5/3 spectrum” is generally observed in turbulence. However, for high order structure functions the difference with the Kolmogorov scaling is significant, and the breakdown of the statistical self-similarity is clear. This behavior, and the lack of universality of the \( C_n \) constants, are related with the phenomenon of intermittency in turbulence. This is an important area of research in this field, and a major goal of the modern theory of turbulence is to understand what is really universal in the inertial range.

### 1.5 See also

- Astronomical seeing
- Atmospheric dispersion modeling
- Chaos theory
- Clear-air turbulence
- Constructal theory
- Downdrafts
- Eddy covariance
- Fluid dynamics
  - Darcy–Weisbach equation
  - Eddy
  - Navier-Stokes equations
  - Large eddy simulation
  - Poiseuille’s law
  - Lagrangian coherent structure
  - Turbulence kinetic energy
- Mesocyclones
- Navier-Stokes existence and smoothness
- Reynolds Number
- Swing bowling
- Taylor microscale
- Turbulence modeling
- Velocimetry
- Vortex
- Vortex generator
- Wake turbulence
- Wave turbulence
- Wingtip vortices
- Wind tunnel
- Different types of boundary conditions in fluid dynamics

### 1.6 References and notes


[3] weizmann.ac.il


[8] scholarpedia.org; G. Falkovich, Scholarpedia, “Cascade and scaling”.


1.7 Further reading

1.7.1 General


1.7.2 Original scientific research papers and classic monographs


1.8 External links

- Center for Turbulence Research, Stanford University
- Scientific American article
- Air Turbulence Forecast
- international CFD database iCFDdatabase
- Turbulent flow in a pipe on YouTube
- Fluid Mechanics website with movies, Q&A, etc
- Johns Hopkins public database with direct numerical simulation data
Chapter 2

Turbulence modeling

Turbulence modeling is the construction and use of a model to predict the effects of turbulence. Averaging is often used to simplify the solution of the governing equations of turbulence, but models are needed to represent scales of the flow that are not resolved.

2.1 Closure problem

A closure problem arises in the Reynolds-averaged Navier-Stokes (RANS) equation because of the nonlinear term $-\rho \bar{u}_i \bar{v}_j$ from the convective acceleration, known as the Reynolds stress,

$$ R_{ij} = -\rho \frac{\partial \bar{u}_i}{\partial x_j} $$

Closing the RANS equation requires modeling the Reynolds stress $R_{ij}$.

2.2 Eddy viscosity

Joseph Boussinesq was the first practitioner of this (i.e. modeling the Reynolds stress), introducing the concept of eddy viscosity. In 1887 Boussinesq proposed relating the turbulence stresses to the mean flow to close the system of equations. Here the Boussinesq hypothesis is applied to model the Reynolds stress term. Note that a new proportionality constant $\nu_t > 0$, the turbulence eddy viscosity, has been introduced. Models of this type are known as eddy viscosity models or EVM’s.

$$ -\rho \bar{u}_i \bar{v}_j = \nu_t \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{v}_j}{\partial x_i} \right) - \frac{2}{3} K \delta_{ij} $$

Which can be written in shorthand as

$$ -\rho \bar{u}_i \bar{v}_j = 2 \nu_t S_{ij} - \frac{2}{3} K \delta_{ij} $$

where $S_{ij}$ is the mean rate of strain tensor

$\nu_t$ is the turbulence eddy viscosity

$K = \frac{1}{2} \bar{u}_i \bar{u}_i$ is the turbulence kinetic energy

$\delta_{ij}$ is the Kronecker delta.

In this model, the additional turbulence stresses are given by augmenting the molecular viscosity with an eddy viscosity. This can be a simple constant eddy viscosity (which works well for some free shear flows such as axisymmetric jets, 2-D jets, and mixing layers).

2.3 Prandtl’s mixing-length concept

Later, Ludwig Prandtl introduced the additional concept of the mixing length, along with the idea of a boundary layer. For wall-bounded turbulent flows, the eddy viscosity must vary with distance from the wall, hence the addition of the concept of a ‘mixing length’. In the simplest wall-bounded flow model, the eddy viscosity is given by the equation:

$$ \nu_t = \frac{1}{l_m} \frac{\partial u}{\partial y}^2 $$

where:

$$ \frac{\partial u}{\partial y} = \frac{l_m}{\nu_t} $$

This simple model is the basis for the "law of the wall", which is a surprisingly accurate model for wall-bounded, attached (not separated) flow fields with small pressure gradients.

More general turbulence models have evolved over time, with most modern turbulence models given by field equations similar to the Navier-Stokes equations.

2.4 Smagorinsky model for the sub-grid scale eddy viscosity

Among many others, Joseph Smagorinsky (1964) proposed a useful formula for the eddy viscosity in numerical models, based on the local derivatives of the velocity field and the local grid size:
\[ \nu_t = \Delta x \Delta y \sqrt{\left( \frac{\partial u}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial y} \right)^2 + \frac{1}{2} \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)^2} \]

### 2.5 Spalart–Allmaras, \(k-\epsilon\) and \(k-\omega\) models

The Boussinesq hypothesis is employed in the Spalart–Allmaras (S–A), \(k-\epsilon\) (\(k\)-epsilon), and \(k-\omega\) (\(k\)-omega) models and offers a relatively low cost computation for the turbulence viscosity \(\nu_t\). The S–A model uses only one additional equation to model turbulence viscosity transport, while the \(k\) models use two.

### 2.6 Common models

The following is a list of commonly employed models in modern engineering applications.

- Spalart–Allmaras (S–A)
- \(k-\epsilon\) (\(k\)-epsilon)
- \(k-\omega\) (\(k\)-omega)
- SST (Menter’s Shear Stress Transport)
- Reynolds stress equation model

### 2.7 References

#### 2.7.1 Notes


#### 2.7.2 Other

Chapter 3

Reynolds stress equation model

Reynolds stress equation model (RSM), also known as second order or second moment closure model is the most complex classical turbulence model. Several shortcomings of k-epsilon turbulence model were observed when it was attempted to predict flows with complex strain fields or substantial body forces. Under those conditions the individual Reynolds stresses were not found to be accurate while using formula

\[
-u_i'u_j' = \mu \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \frac{2}{3} \rho k \delta_{ij} = 2 \mu t E_{ij} - \frac{2}{3} \rho k \delta_{ij}
\]

The equation for the transport of kinematic Reynolds stress \( R_{ij} = u_i'u_j' \) is

\[
\frac{\partial R_{ij}}{\partial t} = D_{ij} + P_{ij} + \Pi_{ij} + \Omega_{ij} - \epsilon_{ij}
\]

Rate of change of \( R_{ij} \) + Transport of \( R_{ij} \) by convection = Transport of \( R_{ij} \) by diffusion + Rate of production of \( R_{ij} \) + Transport of \( R_{ij} \) due to turbulent pressure-strain interactions + Transport of \( R_{ij} \) due to rotation + Rate of dissipation of \( R_{ij} \).

The six partial differential equations above represent six independent Reynolds stresses. The models that we need to solve the above equation are derived from the work of Launder, Rodi and Reece (1975).

3.1 Production term

The Production term that is used in CFD computations with Reynolds stress transport equations is

\[
P_{ij} = - \left( R_{im} \frac{\partial U_i}{\partial x_m} + R_{jm} \frac{\partial U_j}{\partial x_m} \right)
\]

3.2 Pressure-strain interactions

Pressure-strain interactions affect the Reynolds stresses by two different physical processes: pressure fluctuations due to eddies interacting with one another and pressure fluctuation of an eddy with a region of different mean velocity. This redistributes energy among normal Reynolds stresses and thus makes them more isotropic. It also reduces the Reynolds shear stresses.

It is observed that the wall effect increases the anisotropy of normal Reynolds stresses and decreases Reynolds shear stresses. A comprehensive model that takes into account these effects was given by Launder and Rodi (1975).

3.3 Dissipation term

The modelling of dissipation rate \( \epsilon_{ij} \) assumes that the small dissipative eddies are isotropic. This term affects only the normal Reynolds stresses.

\[
\epsilon_{ij} = 2/3 \epsilon \delta_{ij}
\]

where \( \epsilon \) is dissipation rate of turbulent kinetic energy, and \( \delta_{ij} = 1 \) when \( i = j \) and 0 when \( i \neq j \)

3.4 Diffusion term

The modelling of diffusion term \( D_{ij} \) is based on the assumption that the rate of transport of Reynolds stresses by diffusion is proportional to the gradients of Reynolds stresses. The simplest form of \( D_{ij} \) that is followed by commercial CFD codes is

\[
D_{ij} = \frac{\partial}{\partial x_m} \left( \nu_k \frac{\partial U_i}{\partial x_m} \right) = div \left( \nu_k \nabla (R_{ij}) \right)
\]

where \( \nu_k = C_\mu k^2/\sigma_k \), \( \sigma_k = 1.0 \) and \( C_\mu = 0.9 \)

3.5 Pressure-strain correlation term

The pressure-strain correlation term promotes isotropy of the turbulence by redistributing energy amongst the normal Reynolds stresses. The pressure-strain interactions is the most important term to model correctly. Their effect on Reynolds stresses is caused by pressure fluctuations due to interaction of eddies with each other and pressure fluctuations due to interaction of an eddy with region of flow having different mean velocity. The correction term is given as

\[
\Pi_{ij} = -C_1 \frac{k}{\epsilon} \left( R_{ij} - \frac{2}{3} k \delta_{ij} \right) - C_2 \left( P_{ij} - \frac{2}{3} P \delta_{ij} \right)
\]
3.6 Rotational term

The rotational term is given as \[^{[4]}\]

\[ \Omega_{ij} = -2\omega_k (R_{jm}e_{ikm} + R_{im}e_{jkm}) \]

here \( \omega_k \) is the rotation vector, \( e_{ijk} = 1 \) if \( i,j,k \) are in cyclic order and are different, \( e_{ijk} = -1 \) if \( i,j,k \) are in anti-cyclic order and are different and \( e_{ijk} = 0 \) in case any two indices are same.

3.7 Advantages of RSM

1) Compared with k-ε model, it is simple because of the use of an isotropic eddy viscosity.
2) It is the most general of all turbulence models and work reasonably well for a large number of engineering flows.
3) It requires only the initial and/or boundary conditions to be supplied.
4) Since the production terms need not be modelled, it can selectively damp the stresses due to buoyancy, curvature effects etc.

3.8 Disadvantages of RSM

1) It requires very large computing costs.
2) It is not very widely validated as the k-ε model and mixing length models.
3) Due to identical problems with the \( \epsilon \)-equation modelling, it performs just as poorly as the k-ε model in some problems.
4) Because of being isotropic, it is not good in predicting normal stresses and is unable to account for irrotational strains.

3.9 See also

- Reynolds Stress
- Isotropy
- Turbulence Modeling
- Eddy
- k-epsilon turbulence model

3.10 See also

- k-epsilon turbulence model
- Mixing length model

3.11 References


3.12 Bibliography

- “Turbulence : An Introduction for Scientists and Engineers” By P.A. Davidson.
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Chapter 4

Boundary layer

For the anatomical structure, see Boundary layer of uterus.

In physics and fluid mechanics, a boundary layer is the

layer of fluid in the immediate vicinity of a bounding surface where the effects of viscosity are significant. In the Earth’s atmosphere, the atmospheric boundary layer is the air layer near the ground affected by diurnal heat, moisture or momentum transfer to or from the surface. On an aircraft wing the boundary layer is the part of the flow close to the wing, where viscous forces distort the surrounding non-viscous flow. See Reynolds number.

Laminar boundary layers can be loosely classified according to their structure and the circumstances under which they are created. The thin shear layer which develops on an oscillating body is an example of a Stokes boundary layer, while the Blasius boundary layer refers to the well-known similarity solution near an attached flat plate held in an oncoming unidirectional flow. When a fluid rotates and viscous forces are balanced by the Coriolis effect (rather than convective inertia), an Ekman layer forms. In the theory of heat transfer, a thermal boundary layer occurs. A surface can have multiple types of boundary layer simultaneously.

4.1 Aerodynamics

The aerodynamic boundary layer was first defined by Ludwig Prandtl in a paper presented on August 12, 1904 at the third International Congress of Mathematicians in Heidelberg, Germany. It simplifies the equations of fluid flow by dividing the flow field into two areas: one inside the boundary layer, dominated by viscosity and creating the majority of drag experienced by the boundary body; and one outside the boundary layer, where viscosity can be neglected without significant effects on the solution. This allows a closed-form solution for the flow in both areas, a significant simplification of the full Navier–Stokes equations. The majority of the heat transfer to and from a body also takes place within the boundary layer, again allowing the equations to be simplified in the flow field outside the boundary layer. The pressure distribution throughout the boundary layer in the direction normal to the surface (such as an airfoil) remains constant throughout the boundary layer, and is the same as on the surface itself.

The thickness of the velocity boundary layer is normally defined as the distance from the solid body at which the viscous flow velocity is 99% of the freestream velocity (the surface velocity of an inviscid flow). Displacement Thickness is an alternative definition stating that the boundary layer represents a deficit in mass flow compared to inviscid flow with slip at the wall. It is the distance by which the wall would have to be displaced in the inviscid case to give the same total mass flow as the viscous case. The no-slip condition requires the flow velocity at the surface of a solid object be zero and the fluid temperature be equal to the temperature of the surface. The flow velocity will then increase rapidly within the boundary layer, governed by the boundary layer equations, below.

The thermal boundary layer thickness is similarly the distance from the body at which the temperature is 99% of the temperature found from an inviscid solution. The ratio of the two thicknesses is governed by the Prandtl number. If the Prandtl number is 1, the two boundary layers
are the same thickness. If the Prandtl number is greater than 1, the thermal boundary layer is thinner than the velocity boundary layer. If the Prandtl number is less than 1, which is the case for air at standard conditions, the thermal boundary layer is thicker than the velocity boundary layer.

In high-performance designs, such as gliders and commercial aircraft, much attention is paid to controlling the behavior of the boundary layer to minimize drag. Two effects have to be considered. First, the boundary layer adds to the effective thickness of the body, through the displacement thickness, hence increasing the pressure drag. Secondly, the shear forces at the surface of the wing create skin friction drag.

At high Reynolds numbers, typical of full-sized aircraft, it is desirable to have a laminar boundary layer. This results in a lower skin friction due to the characteristic velocity profile of laminar flow. However, the boundary layer inevitably thickens and becomes less stable as the flow develops along the body, and eventually becomes turbulent, the process known as boundary layer transition. One way of dealing with this problem is to suck the boundary layer away through a porous surface (see Boundary layer suction). This can reduce drag, but is usually impractical due to its mechanical complexity and the power required to move the air and dispose of it. Natural laminar flow techniques push the boundary layer transition aft by reshaping the aerofoil or fuselage so that its thickest point is more aft and less thick. This reduces the velocities in the leading part and the same Reynolds number is achieved with a greater length.

At lower Reynolds numbers, such as those seen with model aircraft, it is relatively easy to maintain laminar flow. This gives low skin friction, which is desirable. However, the same velocity profile which gives the laminar boundary layer its low skin friction also causes it to be badly affected by adverse pressure gradients. As the pressure begins to recover over the rear part of the wing chord, a laminar boundary layer will tend to separate from the surface. Such flow separation causes a large increase in the pressure drag, since it greatly increases the effective size of the wing section. In these cases, it can be advantageous to deliberately trip the boundary layer into turbulence at a point prior to the location of laminar separation, using a turbulator. The fuller velocity profile of the turbulent boundary layer allows it to sustain the adverse pressure gradient without separating. Thus, although the skin friction is increased, overall drag is decreased. This is the principle behind the dimpling on golf balls, as well as vortex generators on aircraft. Special wing sections have also been designed which tailor the pressure recovery so laminar separation is reduced or even eliminated. This represents an optimum compromise between the pressure drag from flow separation and skin friction from induced turbulence.

When using half-models in wind tunnels, a peniche is sometimes used to reduce or eliminate the effect of the boundary layer.

4.2 Naval architecture

Many of the principles that apply to aircraft also apply to ships, submarines, and offshore platforms.

For ships, unlike aircraft, one deals with incompressible flows, where change in water density is negligible (a pressure rise close to 1000kPa leads to a change of only 2–3 kg/m³). This field of fluid dynamics is called hydrodynamics. A ship engineer designs for hydrodynamics first, and for strength only later. The boundary layer development, breakdown, and separation become critical because the high viscosity of water produces high shear stresses. Another consequence of high viscosity is the slip stream effect, in which the ship moves like a spear tearing through a sponge at high velocity.

4.3 Boundary layer equations

The deduction of the boundary layer equations was one of the most important advances in fluid dynamics (Anderson, 2005). Using an order of magnitude analysis, the well-known governing Navier–Stokes equations of viscous fluid flow can be greatly simplified within the boundary layer. Notably, the characteristic of the partial differential equations (PDE) becomes parabolic, rather than the elliptical form of the full Navier–Stokes equations. This greatly simplifies the solution of the equations. By making the boundary layer approximation, the flow is divided into an inviscid portion (which is easy to solve by a number of methods) and the boundary layer, which is governed by an easier to solve PDE. The continuity and Navier–Stokes equations for a two-dimensional steady incompressible flow in Cartesian coordinates are given by

\[
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0
\]

\[
u \left( \frac{\partial u}{\partial x} + \frac{1}{\rho} \frac{\partial p}{\partial x} \right) = -\frac{1}{\rho} \frac{\partial p}{\partial x} + \frac{\partial^2 u}{\partial y^2}
\]

where \( u \) and \( v \) are the velocity components, \( \rho \) is the density, \( p \) is the pressure, and \( \nu \) is the kinematic viscosity of the fluid at a point.

The approximation states that, for a sufficiently high Reynolds number the flow over a surface can be divided into an outer region of inviscid flow unaffected by viscosity (the majority of the flow), and a region close to the surface where viscosity is important (the boundary layer).
Let \( u \) and \( v \) be streamwise and transverse (wall normal) velocities respectively inside the boundary layer. Using scale analysis, it can be shown that the above equations of motion reduce within the boundary layer to become

\[
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0
\]

\[
\frac{u}{\partial x} + v \frac{\partial u}{\partial y} = -\frac{1}{\rho} \frac{\partial p}{\partial x} + \nu \frac{\partial^2 u}{\partial y^2}
\]

and if the fluid is incompressible (as liquids are under standard conditions):

\[
\frac{1}{\rho} \frac{\partial p}{\partial y} = 0
\]

The asymptotic analysis also shows that \( v \), the wall normal velocity, is small compared with \( u \) the streamwise velocity, and that variations in properties in the streamwise direction are generally much lower than those in the wall normal direction.

Since the static pressure \( p \) is independent of \( y \), then pressure at the edge of the boundary layer is the pressure throughout the boundary layer at a given streamwise position. The external pressure may be obtained through an application of Bernoulli’s equation. Let \( u_0 \) be the fluid velocity outside the boundary layer, where \( u \) and \( u_0 \) are both parallel. This gives upon substituting for \( p \) the following result

\[
u \frac{u}{\partial x} + v \frac{\partial u}{\partial y} = u_0 \frac{\partial u}{\partial x} + \nu \frac{\partial^2 u}{\partial y^2}
\]

with the boundary condition

\[
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0
\]

For a flow in which the static pressure \( p \) also does not change in the direction of the flow then

\[
\frac{\partial p}{\partial x} = 0
\]

so \( u_0 \) remains constant.

Therefore, the equation of motion simplifies to become

\[
u \frac{u}{\partial x} + v \frac{\partial u}{\partial y} = \nu \frac{\partial^2 u}{\partial y^2}
\]

These approximations are used in a variety of practical flow problems of scientific and engineering interest. The above analysis is for any instantaneous laminar or turbulent boundary layer, but is used mainly in laminar flow studies since the mean flow is also the instantaneous flow because there are no velocity fluctuations present.

### 4.4 Turbulent boundary layers

The treatment of turbulent boundary layers is far more difficult due to the time-dependent variation of the flow properties. One of the most widely used techniques in which turbulent flows are tackled is to apply Reynolds decomposition. Here the instantaneous flow properties are decomposed into a mean and fluctuating component.

Applying this technique to the boundary layer equations gives the full turbulent boundary layer equations not often given in literature:

\[
\frac{\partial \bar{u}}{\partial x} + \frac{\partial \bar{u}}{\partial y} = 0
\]

\[
\frac{\partial \bar{u}}{\partial x} + \frac{\partial \bar{u}}{\partial y} = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x} + \nu \left( \frac{\partial^2 \bar{u}}{\partial x^2} + \frac{\partial^2 \bar{u}}{\partial y^2} \right) - \frac{\partial}{\partial y} \left( \bar{u}' \bar{v}' \right) - \frac{\partial}{\partial x} \left( \bar{u}' \bar{u}' \right)
\]

Using the same order-of-magnitude analysis as for the instantaneous equations, these turbulent boundary layer equations generally reduce to become in their classical form:

\[
\frac{\partial \bar{u}}{\partial x} + \frac{\partial \bar{u}}{\partial y} = 0
\]

\[
\frac{\partial \bar{u}}{\partial x} + \frac{\partial \bar{u}}{\partial y} = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x} + \nu \frac{\partial^2 \bar{u}}{\partial y^2} - \frac{\partial}{\partial y} \left( \bar{u}' \bar{v}' \right)
\]

\[
\frac{\partial \bar{p}}{\partial y} = 0
\]

The additional term \( \bar{u}' \bar{v}' \) in the turbulent boundary layer equations is known as the Reynolds shear stress and is unknown a priori. The solution of the turbulent boundary layer equations therefore necessitates the use of a turbulence model, which aims to express the Reynolds shear stress in terms of known flow variables or derivatives. The lack of accuracy and generality of such models is a major obstacle in the successful prediction of turbulent flow properties in modern fluid dynamics.

A laminar sub-layer exists in the turbulent zone; it occurs due to those fluid molecules which are still in the very proximity of the surface, where the shear stress is maximum and the velocity of fluid molecules is zero.

### 4.5 Heat and mass transfer

In 1928, the French engineer André Lévêque observed that convective heat transfer in a flowing fluid is affected only by the velocity values very close to the surface.\cite{1,2}

For flows of large Prandtl number, the temperature/mass transition from surface to freestream temperature takes
place across a very thin region close to the surface. Therefore, the most important fluid velocities are those inside this very thin region in which the change in velocity can be considered linear with normal distance from the surface. In this way, for

\[
u(y) = u_0 \left(1 - \frac{(y-h)^2}{h^2}\right) = u_0 \frac{y}{h} \left(2 - \frac{y}{h}\right),
\]

when \(y \to 0\), then

\[
u(y) \approx 2u_0 \frac{y}{h} = \theta y
\]

where \(\theta\) is the tangent of the Poiseuille parabola intersecting the wall. Although Lévéque's solution was specific to heat transfer into a Poiseuille flow, his insight helped lead other scientists to an exact solution of the thermal boundary-layer problem.\[3\] Schuh observed that in a boundary-layer, \(\nu\) is again a linear function of \(y\), but that in this case, the wall tangent is a function of \(x\).\[4\] He expressed this with a modified version of Lévéque's profile,

\[
u(y) = \theta(x)y
\]

This results in a very good approximation, even for low \(Pr\) numbers, so that only liquid metals with \(Pr\) much less than 1 cannot be treated this way.\[3\] In 1962, Kestin and Persen published a paper describing solutions for heat transfer when the thermal boundary layer is contained entirely within the momentum layer and for various wall temperature distributions.\[5\] For the problem of a flat plate with a temperature jump at \(x = x_0\), they propose a substitution that reduces the parabolic thermal boundary-layer equation to an ordinary differential equation. The solution to this equation, the temperature at any point in the fluid, can be expressed as an incomplete gamma function.\[2\] Schlichting proposed an equivalent substitution that reduces the thermal boundary-layer equation to an ordinary differential equation whose solution is the same incomplete gamma function.\[6\]

### 4.6 Convective transfer constants from boundary layer analysis

Paul Richard Heinrich Blasius derived an exact solution to the above laminar boundary layer equations.\[7\] The thickness of the boundary layer \(\delta\) is a function of the Reynolds number for laminar flow.

\[
\delta \approx \frac{0.03x}{\sqrt{Re}}
\]

\(\delta\) is the thickness of the boundary layer: the region of flow where the velocity is less than 99% of the far field velocity \(v_\infty\); \(x\) is position along the semi-infinite plate, and \(Re\) is the Reynolds Number given by \(\rho v_\infty x/\mu\) (\(\rho\) is density and \(\mu\) is dynamic viscosity).

The Blasius solution uses boundary conditions in a dimensionless form:

\[
\begin{align*}
\frac{v_\nu - v_\nu}{v_\nu} &= \frac{v_\nu}{v_\nu} = 0 \text{ at } y = 0 \\
\frac{v_\nu - v_\nu}{v_\nu} &= \frac{v_\nu}{v_\nu} = 1 \text{ at } y = \infty \text{ and } x = 0
\end{align*}
\]

Note that in many cases, the no-slip boundary condition holds that \(v_S\), the fluid velocity at the surface of the plate equals the velocity of the plate at all locations. If the plate is not moving, then \(v_S = 0\). A much more complicated derivation is required if fluid slip is allowed.\[8\]

In fact, the Blasius solution for laminar velocity profile in the boundary layer above a semi-infinite plate can be easily extended to describe Thermal and Concentration boundary layers for heat and mass transfer respectively. Rather than the differential x-momentum balance (equation of motion), this uses a similarly derived Energy and Mass balance:

**Energy:**

\[
v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y} = \frac{k}{\rho C_P} \frac{\partial^2 T}{\partial y^2}
\]

**Mass:**

\[
v_x \frac{\partial c_A}{\partial x} + v_y \frac{\partial c_A}{\partial y} = D_{AB} \frac{\partial^2 c_A}{\partial y^2}
\]

For the momentum balance, kinematic viscosity \(\nu\) can be considered to be the momentum diffusivity. In the energy balance this is replaced by thermal diffusivity \(\alpha = k/\rho C_P\), and by mass diffusivity \(D_{AB}\) in the mass balance. In thermal diffusivity of a substance, \(k\) is its thermal conductivity, \(\rho\) is its density and \(C_P\) is its heat capacity. Subscript AB denotes diffusivity of species A diffusing into species B.
Under the assumption that $\alpha = D_{AB} = \nu$, these equations become equivalent to the momentum balance. Thus, for Prandtl number $Pr = \nu/\alpha = 1$ and Schmidt number $Sc = \nu/D_{AB} = 1$ the Blasius solution applies directly.

Accordingly, this derivation uses a related form of the boundary conditions, replacing $v$ with $T$ or $c_A$ (absolute temperature or concentration of species A). The subscript S denotes a surface condition.

\[
\frac{v_c-v_s}{v_{\infty}-v_s} = \frac{T-T_s}{T_{\infty}-T_s} = \frac{c_{A,c}-c_{A,s}}{c_{A,\infty}-c_{A,s}} = 0 \quad \text{at } y = 0
\]

\[
\frac{v_c-v_s}{x} = \frac{T-T_s}{T_{\infty}-T_s} = \frac{c_{A,c}-c_{A,s}}{c_{A,\infty}-c_{A,s}} = 1 \quad \text{at } y = \infty 	ext{ and } x = 0
\]

Using the streamline function Blasius obtained the following solution for the shear stress at the surface of the plate.

\[
\tau_0 = \left( \frac{\partial T}{\partial y} \right)_{y=0} = 0.332 \frac{v_c}{x} Re^{1/2}
\]

And via the boundary conditions, it is known that

\[
\frac{v_{\infty}-v_s}{v_{\infty}-v_s} = \frac{T_{\infty}-T_s}{T_{\infty}-T_s} = \frac{c_{A,\infty}-c_{A,s}}{c_{A,\infty}-c_{A,s}}
\]

We are given the following relations for heat/mass flux out of the surface of the plate

\[
\left( \frac{\partial T}{\partial y} \right)_{y=0} = 0.332 \frac{T_{\infty}-T_s}{x} Re^{1/2}
\]

\[
\left( \frac{\partial c}{\partial y} \right)_{y=0} = 0.332 \frac{c_{A,\infty}-c_{A,s}}{x} Re^{1/2}
\]

So for $Pr = Sc = 1$

\[
\delta_{c} = \delta_{T} = \frac{5.9 x}{V Re^{1/3}}
\]

Where $\delta_T$, $\delta_c$ are the regions of flow where $T$ and $c_A$ are less than 99% of their far field values.[9]

Because the Prandtl number of a particular fluid is not often unity, German engineer E. Polhausen who worked with Ludwig Prandtl attempted to empirically extend these equations to apply for $Pr \neq 1$. His results can be applied to $Sc$ as well.[10] He found that for Prandtl number greater than 0.6, the thermal boundary layer thickness was approximately given by:

\[
\frac{\delta_T}{x} = Pr^{1/3} \text{ and therefore } \frac{\delta_c}{x} = Sc^{1/3}
\]

From this solution, it is possible to characterize the convective heat/mass transfer constants based on the region of boundary layer flow. Fourier’s law of conduction and Newton’s Law of Cooling are combined with the flux term derived above and the boundary layer thickness.

\[
\frac{q}{A} = -k \left( \frac{\partial T}{\partial y} \right)_{y=0} = h_x (T_s - T_{\infty})
\]

\[
h_x = 0.332 \frac{k}{x} Re^{1/2} Pr^{1/3}
\]

This gives the local convective constant $h_x$ at one point on the semi-infinite plane. Integrating over the length of the plate gives an average

\[
h_{L} = 0.664 \frac{k}{x} Re^{1/2} Pr^{1/3}
\]

Following the derivation with mass transfer terms ($k =

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{thermalboundarylayer.png}
\caption{Plot showing the relative thickness in the Thermal boundary layer versus the Velocity boundary layer (in red) for various Prandtl Numbers. For $Pr = 1$, the two are equal.}
\end{figure}

### 4.7 Boundary layer turbine

This effect was exploited in the Tesla turbine, patented by Nikola Tesla in 1913. It is referred to as a bladeless turbine because it uses the boundary layer effect and not a fluid impinging upon the blades as in a conventional turbine. Boundary layer turbines are also known as cohesion-type turbine, bladeless turbine, and Prandtl layer turbine (after Ludwig Prandtl).

### 4.8 See also

- Boundary layer separation
- Boundary-layer thickness
- Boundary layer suction
- Boundary layer control
- Coandă effect
- Facility for Airborne Atmospheric Measurements
- Logarithmic law of the wall
- Planetary boundary layer
4.10. EXTERNAL LINKS

- Shape factor (boundary layer flow)
- Shear stress

4.9 References


4.10 External links

- National Science Digital Library – Boundary Layer
- Boundary layer separation
- Boundary layer equations: Exact Solutions – from EqWorld
- Jones, T.V. BOUNDARY LAYER HEAT TRANSFER
Chapter 5

Similitude (model)

For other uses, see Similitude (disambiguation).

Similitude is a concept applicable to the testing of engineering models. A model is said to have similitude with the real application if the two share geometric similarity, kinematic similarity and dynamic similarity. Similarity and similitude are interchangeable in this context.

The term dynamic similitude is often used as a catch-all because it implies that geometric and kinematic similitude have already been met.

Similitude’s main application is in hydraulic and aerospace engineering to test fluid flow conditions with scaled models. It is also the primary theory behind many textbook formulas in fluid mechanics.

5.1 Overview

Engineering models are used to study complex fluid dynamics problems where calculations and computer simulations aren’t reliable. Models are usually smaller than the final design, but not always. Scale models allow testing of a design prior to building, and in many cases are a critical step in the development process.

Construction of a scale model, however, must be accompanied by an analysis to determine what conditions it is tested under. While the geometry may be simply scaled, other parameters, such as pressure, temperature or the velocity and type of fluid may need to be altered. Similitude is achieved when testing conditions are created such that the test results are applicable to the real design.

The three conditions required for a model to have similitude with an application.

The following criteria are required to achieve similitude;

- **Geometric similarity** – The model is the same shape as the application, usually scaled.
- **Kinematic similarity** – Fluid flow of both the model and real application must undergo similar time rates of change motions. (fluid streamlines are similar)
- **Dynamic similarity** – Ratios of all forces acting on corresponding fluid particles and boundary surfaces in the two systems are constant.

To satisfy the above conditions the application is analyzed;

1. All parameters required to describe the system are identified using principles from continuum mechanics.
2. Dimensional analysis is used to express the system with as few independent variables and as many dimensionless parameters as possible.
3. The values of the dimensionless parameters are held to be the same for both the scale model and application. This can be done because they are dimensionless and will ensure dynamic similitude between the model and the application. The resulting equations are used to derive scaling laws which dictate model testing conditions.

It is often impossible to achieve strict similitude during a model test. The greater the departure from the application’s operating conditions, the more difficult achieving similitude is. In these cases some aspects of similitude may be neglected, focusing on only the most important parameters.

The design of marine vessels remains more of an art than a science in large part because dynamic similitude is especially difficult to attain for a vessel that is partially submerged: a ship is affected by wind forces in the air above it, by hydrodynamic forces within the water under it, and especially by wave motions at the interface between the water and the air. The scaling requirements for each of these phenomena differ, so models cannot replicate what happens to a full sized vessel nearly so well as can be done for an aircraft or submarine—each of which operates entirely within one medium.

Similitude is a term used widely in fracture mechanics relating to the strain life approach. Under given loading conditions the fatigue damage in an un-notched specimen is comparable to that of a notched specimen. Similitude suggests that the component fatigue life of the two objects will also be similar.

5.2 An example

Consider a submarine modeled at 1/40th scale. The application operates in sea water at 0.5 °C, moving at 5 m/s. The model will be tested in fresh water at 20 °C. Find the power required for the submarine to operate at the stated speed.

A free body diagram is constructed and the relevant relationships of force and velocity are formulated using techniques from continuum mechanics. The variables which describe the system are:

This example has five independent variables and three fundamental units. The fundamental units are: metre, kilogram, second.[1]

Invoking the Buckingham π theorem shows that the system can be described with two dimensionless numbers and one independent variable.[2]

Dimensional analysis is used to re-arrange the units to form the Reynolds number ( \( R_e \) ) and Pressure coefficient ( \( C_p \) ). These dimensionless numbers account for all the variables listed above except \( F \), which will be the test measurement. Since the dimensionless parameters will stay constant for both the test and the real application, they will be used to formulate scaling laws for the test.

**Scaling laws:**

\[
R_e = \left( \frac{\rho VL}{\mu} \right) \\
\rightarrow V_{model} = V_{application} \times \left( \frac{\rho_a}{\rho_m} \right) \times \left( \frac{L_a}{L_m} \right)
\]

\[
C_p = \left( \frac{2\Delta p}{\rho V^2} \right), F = \Delta p L^2 \rightarrow F_{application} = F_{model} \times \left( \frac{\rho_a}{\rho_m} \right) \times \left( \frac{V_a}{V_m} \right)
\]

The pressure ( \( p \) ) is not one of the five variables, but the force ( \( F \) ) is. The pressure difference (\( \Delta p \)) has thus been replaced with (\( F/L^2 \)) in the pressure coefficient. This gives a required test velocity of:

\[
V_{model} = V_{application} \times 21.9
\]

A model test is then conducted at that velocity and the force that is measured in the model (\( F_{model} \)) is then scaled to find the force that can be expected for the real application (\( F_{application} \)):

\[
F_{application} = F_{model} \times 3.44
\]

The power \( P \) in watts required by the submarine is then:

\[
P[W] = F_{application} \times V_{application} = F_{model}[N] \times 17.2 \text{ m/s}
\]

Note that even though the model is scaled smaller, the water velocity needs to be increased for testing. This remarkable result shows how similitude in nature is often counterintuitive.

5.3 Typical applications

See also: List of dimensionless numbers

Similitude has been well documented for a large number of engineering problems and is the basis of many textbook formulas and dimensionless quantities. These formulas and quantities are easy to use without having to repeat the laborious task of dimensional analysis and formula derivation. Simplification of the formulas (by neglecting some aspects of similitude) is common, and needs to be reviewed by the engineer for each application.

Similitude can be used to predict the performance of a new design based on data from an existing, similar design. In this case, the model is the existing design. Another use of similitude and models is in validation of computer simulations with the ultimate goal of eliminating the need for physical models altogether.
Another application of similitude is to replace the operating fluid with a different test fluid. Wind tunnels, for example, have trouble with air liquefying in certain conditions so helium is sometimes used. Other applications may operate in dangerous or expensive fluids so the testing is carried out in a more convenient substitute. Some common applications of similitude and associated dimensionless numbers;

5.7 External links
- MIT open courseware lecture notes on Similitude for marine engineering (pdf file)

5.4 Notes

[1] In the SI system of units newtons can be expressed in terms of kg·m/s².

[2] 5 variables - 3 fundamental units => 2 dimensionless numbers.

5.5 See also
- Dimensionless number
- Buckingham π theorem
- Dimensional analysis
- MKS system of fundamental units
- Dynamic similarity (Reynolds and Womersley numbers)
- Similitude of ship models

5.6 References
Chapter 6

Lagrangian and Eulerian specification of the flow field

This article is about fluid mechanics. For the use of generalized coordinates in classical mechanics, see generalized coordinates, Lagrangian mechanics and Hamiltonian mechanics.

In fluid dynamics and finite-deformation plasticity the Lagrangian specification of the flow field is a way of looking at fluid motion where the observer follows an individual fluid parcel as it moves through space and time.\(^1\)\(^2\) Plotting the position of an individual parcel through time gives the pathline of the parcel. This can be visualized as sitting in a boat and drifting down a river.

The Eulerian specification of the flow field is a way of looking at fluid motion that focuses on specific locations in the space through which the fluid flows as time passes.\(^1\)\(^2\) This can be visualized by sitting on the bank of a river and watching the water pass the fixed location.

The Lagrangian and Eulerian specifications of the flow field are sometimes loosely denoted as the Lagrangian and Eulerian frame of reference. However, in general both the Lagrangian and Eulerian specification of the flow field can be applied in any observer’s frame of reference, and in any coordinate system used within the chosen frame of reference.

6.1 Description

In the Eulerian specification of the flow field, the flow quantities are depicted as a function of position \(x\) and time \(t\). Specifically, the flow is described by a function

\[ v(x, t) \]

giving the flow velocity at position \(x\) at time \(t\).

On the other hand, in the Lagrangian specification, individual fluid parcels are followed through time. The fluid parcels are labelled by some (time-independent) vector field \(a\). (Often, \(a\) is chosen to be the center of mass of the parcels at some initial time \(t_0\). It is chosen in this particular manner to account for the possible changes of the shape over time. Therefore the center of mass is a good parametrization of the velocity \(v\) of the parcel.)\(^1\) In the Lagrangian description, the flow is described by a function

\[ X(a, t) \]

giving the position of the parcel labeled \(a\) at time \(t\).

The two specifications are related as follows: \(^2\)

\[ v(X(a, t), t) = \frac{\partial X}{\partial t}(a, t) \]

because both sides describe the velocity of the parcel labeled \(a\) at time \(t\).

Within a chosen coordinate system, \(a\) and \(x\) are referred to as the Lagrangian coordinates and Eulerian coordinates of the flow.

6.2 Substantial derivative

Main article: Material derivative

The Lagrangian and Eulerian specifications of the kinematics and dynamics of the flow field are related by the substantial derivative (also called the Lagrangian derivative, convective derivative, material derivative, or particle derivative).\(^1\)

Suppose we have a flow field with Eulerian specification \(v\), and we are also given some function \(F(x, t)\) defined for every position \(x\) and every time \(t\). (For instance, \(F\) could be an external force field, or temperature.) Now one might ask about the total rate of change of \(F\) experienced by a specific flow parcel. This can be computed as

\[
\frac{DF}{Dt} = \frac{\partial F}{\partial t} + (v \cdot \nabla)F
\]
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(where $\nabla$ denotes the gradient with respect to $x$, and the operator $v \cdot \nabla$ is to be applied to each component of $F$.)

This tells us that the total rate of change of the function $F$ as the fluid parcels moves through a flow field described by its Eulerian specification $v$ is equal to the sum of the local rate of change and the convective rate of change of $F$. This is a consequence of the chain rule since we are differentiating the function $F(X(a,t),t)$ with respect to $t$.

Conservation laws for a unit mass have a Lagrangian form, which together with mass conservation produce Eulerian conservation; on the contrary when fluid particle can exchange the quantity (like energy or momentum) only Eulerian conservation law exists, see Falkovich.

6.3 See also

- Contour advection
- Coordinate system
- Equivalent latitude
- Fluid dynamics
- Frame of reference
- Generalized Lagrangian mean
- Lagrangian particle tracking
- Semi-Lagrangian scheme
- Streamlines, streaklines, and pathlines
- Trajectory (fluid mechanics)

6.4 Notes


6.5 References


Chapter 7
Lagrangian mechanics

Lagrangian mechanics is a re-formulation of classical mechanics using the principle of stationary action (also called the principle of least action). It was introduced by the Italian-French mathematician Joseph-Louis Lagrange in 1788.

In Lagrangian mechanics, the trajectory of a system of particles is derived by solving the Lagrange equations in one of two forms, either the Lagrange equations of the first kind, which treat constraints explicitly as extra equations, or the Lagrange equations of the second kind, which incorporate the constraints directly by judicious choice of generalized coordinates. The fundamental lemma of the calculus of variations shows that solving the Lagrange equations is equivalent to finding the path for which the action functional is stationary, a quantity that is the integral of the Lagrangian over time.

The use of generalized coordinates may considerably simplify a system’s analysis. For example, consider a small frictionless bead traveling in a groove. If one is tracking the bead as a particle, calculation of the motion of the bead using Newtonian mechanics would require solving for the time-varying constraint force required to keep the bead in the groove. For the same problem using Lagrangian mechanics, one looks at the path of the groove and chooses a set of independent generalized coordinates that completely characterize the possible motion of the bead. This choice eliminates the need for the constraint force to enter into the resultant system of equations. There are fewer equations since one is not directly calculating the influence of the groove on the bead at a given moment.

7.1 Conceptual framework

7.1.1 Generalized coordinates

Concepts and terminology

For one particle acted on by external forces, Newton’s second law forms a set of 3 second-order ordinary differential equations, one for each dimension. Therefore, the motion of the particle can be completely described by 6 independent variables: 3 initial position coordinates and 3 initial velocity coordinates. Given these, the general solutions to Newton’s second law become particular solutions that determine the time evolution of the particle’s behaviour after its initial state ($t = 0$).

The most familiar set of variables for position $\mathbf{r} = (r_1, r_2, r_3)$ and velocity $\mathbf{v} = (\dot{r}_1, \dot{r}_2, \dot{r}_3)$ are Cartesian coordinates and their time derivatives (i.e. position ($x, y, z$) and velocity ($vx, vy, vz$) components). Determining forces in terms of standard coordinates can be complicated, and usually requires much labour.

An alternative and more efficient approach is to use only as many coordinates as are needed to define the position of the particle, at the same time incorporating the constraints on the system, and writing down kinetic and potential energies. In other words, to determine the number of degrees of freedom the particle has, i.e. the number of possible ways the system can move subject to the constraints (forces that prevent it moving in certain paths). Energies are much easier to write down and calculate than forces, since energy is a scalar while forces are vectors.

These coordinates are generalized coordinates, denoted $q_j$, and there is one for each degree of freedom. Their corresponding time derivatives are the generalized velocities, $\dot{q}_j$. The number of degrees of freedom is usually not equal to the number of spatial dimensions: multi-body systems in 3-dimensional space (such as Barton’s Pendulums, planets in the solar system, or atoms in molecules) can have many more degrees of freedom incorporating rotations as well as translations. This contrasts the number of spatial coordinates used with Newton’s laws above.

Mathematical formulation

The position vector $\mathbf{r}$ in a standard coordinate system (like Cartesian, spherical etc.), is related to the generalized coordinates by some transformation equation:
r = r(qi, t).

where there are as many qi as needed (number of degrees of freedom in the system). Likewise for velocity and generalized velocities.

For example, for a simple pendulum of length ℓ, there is the constraint of the pendulum bob’s suspension (rod/wire/string etc.). The position r depends on the x and y coordinates at time t, that is, r(t)=(x(t), y(t)), however x and y are coupled to each other in a constraint equation (if x changes y must change, and vice versa). A logical choice for a generalized coordinate is the angle of the pendulum from vertical, θ, so we have r = (x(θ), y(θ)) = r(θ), in which θ = 0(t). Then the transformation equation would be

\[
\mathbf{r}(\theta(t)) = (\ell \sin \theta, -\ell \cos \theta)
\]

and so

\[
\mathbf{r}(\theta(t), \dot{\theta}(t)) = (\ell \dot{\theta} \cos \theta, \ell \dot{\theta} \sin \theta)
\]

which corresponds to the one degree of freedom the pendulum has. The term “generalized coordinates” is really a holdover from the period when Cartesian coordinates were the default coordinate system.

In general, from m independent generalized coordinates qi, the following transformation equations hold for a system composed of n particles:

\[
\begin{align*}
\mathbf{r}_1 &= \mathbf{r}_1(q_1, q_2, \cdots, q_m, t) \\
\mathbf{r}_2 &= \mathbf{r}_2(q_1, q_2, \cdots, q_m, t) \\
&\vdots \\
\mathbf{r}_n &= \mathbf{r}_n(q_1, q_2, \cdots, q_m, t)
\end{align*}
\]

where m indicates the total number of generalized coordinates. An expression for the virtual displacement (infinitesimal), δr, of the system for time-independent constraints or “velocity-dependent constraints” is the same form as a total differential

\[
\delta \mathbf{r}_i = \sum_{j=1}^{m} \frac{\partial \mathbf{r}_i}{\partial q_j} \delta q_j,
\]

where j is an integer label corresponding to a generalized coordinate.

The generalized coordinates form a discrete set of variables that define the configuration of a system. The continuum analogue for defining a field are field variables, say φ(r, t), which represents density function varying with position and time.

### 7.1.2 D’Alembert’s principle and generalized forces

D’Alembert’s principle introduces the concept of virtual work due to applied forces \(\mathbf{F}_i\) and inertial forces, acting on a three-dimensional accelerating system of n particles whose motion is consistent with its constraints. Mathematically the virtual work done δW on a particle of mass \(m_i\) through a virtual displacement δri (consistent with the constraints) is:

\[
\delta W = \sum_{j=1}^{n} \sum_{i=1}^{m} (\mathbf{F}_i - m_i \mathbf{a}_i) \cdot \frac{\partial \mathbf{r}_i}{\partial q_j} \delta q_j = 0.
\]

this expression suggests that the applied forces may be expressed as generalized forces, \(Q_j\). Dividing by \(\delta q_j\) gives the definition of a generalized force:

\[
Q_j = \frac{\delta W}{\delta q_j} = \sum_{i=1}^{n} \mathbf{F}_i \cdot \frac{\partial \mathbf{r}_i}{\partial q_j}.
\]

If the forces \(\mathbf{F}_i\) are conservative, there is a scalar potential field \(V\) in which the gradient of \(V\) is the force:

\[
\mathbf{F}_i = -\nabla V \Rightarrow Q_j = -\sum_{i=1}^{n} \nabla V \cdot \frac{\partial \mathbf{r}_i}{\partial q_j} = -\frac{\partial V}{\partial q_j}.
\]

i.e. generalized forces can be reduced to a potential gradient in terms of generalized coordinates. The previous result may be easier to see by recognizing that \(V\) is a function of the \(\mathbf{r}_i\), which are in turn functions of \(q_j\), and then applying the chain rule to the derivative of \(V\) with respect to \(q_j\).

### 7.1.3 Kinetic energy relations

The kinetic energy, \(T\), for the system of particles is defined by

\[
T = \frac{1}{2} \sum_{i=1}^{n} m_i \mathbf{r}_i \cdot \dot{\mathbf{r}}_i.
\]

The partial derivatives of \(T\) with respect to the generalized coordinates \(q_j\) and generalized velocities \(\dot{q}_j\) are
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\[ \frac{\partial T}{\partial q_j} = \sum_{i=1}^{n} m_i \mathbf{r}_i \cdot \frac{\partial \mathbf{r}_i}{\partial q_j} \]

\[ \frac{\partial T}{\partial \dot{q}_j} = \sum_{i=1}^{n} m_i \mathbf{r}_i \cdot \frac{\partial \mathbf{r}_i}{\partial \dot{q}_j} . \]

Because \( q_j \) and \( \dot{q}_j \) are independent variables:

\[ \frac{\partial \mathbf{r}_i}{\partial q_j} = \frac{\partial \mathbf{r}_i}{\partial \dot{q}_j} . \]

Then:

\[ \frac{\partial T}{\partial \dot{q}_j} = \sum_{i=1}^{n} m_i \mathbf{r}_i \cdot \frac{\partial \mathbf{r}_i}{\partial \dot{q}_j} . \]

The total time derivative of this equation is

\[ \frac{d}{dt} \frac{\partial T}{\partial \dot{q}_j} = \sum_{i=1}^{n} m_i \mathbf{r}_i \cdot \frac{\partial \mathbf{r}_i}{\partial q_j} + \sum_{i=1}^{n} m_i \mathbf{r}_i \cdot \frac{\partial \mathbf{r}_i}{\partial \dot{q}_j} = \dot{q}_j + \frac{\partial T}{\partial \dot{q}_j} . \]

resulting in:

\[ S = \int_{t_1}^{t_2} L \; dt. \]

This also contains the dynamics of the system, and has deep theoretical implications (discussed below). Technically, the action is a **functional**, that is, it is a **function** that maps the full Lagrangian function for all times between \( t_1 \) and \( t_2 \) to a scalar value for the action. Its dimensions are the same as angular momentum.

In classical field theory, the physical system is not a set of discrete particles, but rather a continuous field defined over a region of 3d space. Associated with the field is a Lagrangian density \( L(\mathbf{r}, t) \) defined in terms of the field and its derivatives at a location \( \mathbf{r} \). The total Lagrangian is then the integral of the Lagrangian density over 3d space (see volume integral):

\[ L(t) = \int L(\mathbf{r}, t) d^3\mathbf{r} \]

where \( d^3\mathbf{r} \) is a 3d differential volume element, must be used instead. The action becomes an integral over space and time:

\[ S = \int_{t_1}^{t_2} \int L(\mathbf{r}, t) d^3\mathbf{r} dt. \]

7.1.5 Hamilton’s principle of stationary action

Let \( q_0 \) and \( q_1 \) be the coordinates at respective initial and final times \( t_0 \) and \( t_1 \). Using the calculus of variations, it can be shown that Lagrange’s equations are equivalent to **Hamilton’s principle**:

The trajectory of the system between \( t_0 \) and \( t_1 \) has a stationary action \( S \).

By **stationary**, we mean that the action does not vary to first-order from infinitesimal deformations of the trajectory, with the end-points \((q_0, t_0)\) and \((q_1, t_1)\) fixed. Hamilton’s principle can be written as:

\[ \delta S = 0. \]

Thus, instead of thinking about particles accelerating in response to applied forces, one might think of them picking out the path with a stationary action.

Hamilton’s principle is sometimes referred to as the **principle of least action**, however the action functional need only be stationary, not necessarily a maximum or a minimum value. Any variation of the functional gives an increase in the functional integral of the action.

**7.1.4 Lagrangian and action**

The core element of Lagrangian mechanics is the Lagrangian function, which summarizes the dynamics of the entire system in a very simple expression. The physics of analyzing a system is reduced to choosing the most convenient set of generalized coordinates, determining the kinetic and potential energies of the constituents of the system, then writing down the equation for the Lagrangian to use in Lagrange’s equations. It is defined by

\[ L = T - V \]

where \( T \) is the total kinetic energy and \( V \) is the total potential energy of the system.

The next fundamental element is the action \( S \), defined as the time integral of the Lagrangian: \[ S = \int_{t_1}^{t_2} L \; dt. \]
We can use this principle instead of Newton’s Laws as the fundamental principle of mechanics, this allows us to use an integral principle (Newton’s Laws are based on differential equations so they are a differential principle) as the basis for mechanics. However it is not widely stated that Hamilton’s principle is a variational principle only with holonomic constraints, if we are dealing with non-holonomic systems then the variational principle should be replaced with one involving d’Alembert principle of virtual work. Working only with holonomic constraints is the price we have to pay for using an elegant variational formulation of mechanics.

7.2 Lagrange equations of the first kind

Lagrange introduced an analytical method for finding stationary points using the method of Lagrange multipliers, and also applied it to mechanics.

For a system subject to the (holonomic) constraint equation on the generalized coordinates:

\[ F(r_1, r_2, r_3) = A \]

where \( A \) is a constant, then Lagrange’s equations of the first kind are:

\[
\left[ \frac{\partial L}{\partial r_j} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{r}_j} \right) \right] + \lambda \frac{\partial F}{\partial r_j} = 0
\]

where \( \lambda \) is the Lagrange multiplier. By analogy with the mathematical procedure, we can write:

\[
\frac{\delta L}{\delta r_j} + \lambda \frac{\partial F}{\partial r_j} = 0
\]

where

\[
\frac{\delta L}{\delta r_j} = \frac{\partial L}{\partial r_j} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{r}_j} \right)
\]

denotes the variational derivative.

For \( e \) constraint equations \( F_1, F_2, ..., F_e \), there is a Lagrange multiplier for each constraint equation, and Lagrange’s equations of the first kind generalize to:

This procedure does increase the number of equations, but there are enough to solve for all of the multipliers. The number of equations generated is the number of constraint equations plus the number of coordinates, i.e. \( e + m \). The advantage of the method is that (potentially complicated) substitution and elimination of variables linked by constraint equations can be bypassed.

There is a connection between the constraint equations \( F_j \) and the constraint forces \( N_j \) acting in the conservative system (forces are conservative):

\[ N_j = \sum_{i=1}^{e} \lambda_i \frac{\partial F_i}{\partial r_j} \]

which is derived below.

7.3 Lagrange equations of the second kind

7.3.1 Euler–Lagrange equations

For any system with \( m \) degrees of freedom, the Lagrange equations include \( m \) generalized coordinates and \( m \) generalized velocities. Below, we sketch out the derivation of the Lagrange equations of the second kind. In this context, \( V \) is used rather than \( U \) for potential energy and \( T \) replaces \( K \) for kinetic energy. See the references for more detailed and more general derivations.

The equations of motion in Lagrangian mechanics are the Lagrange equations of the second kind, also known as the Euler–Lagrange equations:

\[
\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_j} \right) - \frac{\partial L}{\partial q_j} = 0
\]

where \( j = 1, 2, ..., m \) represents the \( j \)th degree of freedom, \( q_j \) are the generalized coordinates, and \( \dot{q}_j \) are the generalized velocities.

Although the mathematics required for Lagrange’s equations appears significantly more complicated than Newton’s laws, this does point to deeper insights into classical mechanics than Newton’s laws alone: in particular, symmetry and conservation. In practice it’s often easier to solve a problem using the Lagrange equations than Newton’s laws, because the minimum generalized coordinates \( q_i \) can be chosen by convenience to exploit symmetries in the system, and constraint forces are incorporated into the geometry of the problem. There is one Lagrange equation for each generalized coordinate \( q_i \).

For a system of many particles, each particle can have different numbers of degrees of freedom from the others. In each of the Lagrange equations, \( T \) is the total kinetic energy of the system, and \( V \) the total potential energy.

7.3.2 Derivation of Lagrange’s equations
7.3. LAGRANGE EQUATIONS OF THE SECOND KIND

Hamilton’s principle

The Euler–Lagrange equations follow directly from Hamilton’s principle, and are mathematically equivalent. From the calculus of variations, any functional of the form:

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

leads to the general Euler–Lagrange equation for stationary value of \( J \). (see main article for derivation):

\[ \frac{d}{dx} \frac{\partial F}{\partial y'} = \frac{\partial F}{\partial y} \]

Then making the replacements:

\[ x \to t, \quad y \to q, \quad y' \to \dot{q}, \quad F \to L, \quad J \to S \]

yields the Lagrange equations for mechanics. Since mathematically Hamilton’s equations can be derived from Lagrange’s equations (by a Legendre transformation) and Lagrange’s equations can be derived from Newton’s laws, all of which are equivalent and summarize classical mechanics, this means classical mechanics is fundamentally ruled by a variation principle (Hamilton’s principle above).

Generalized forces

For a conservative system, since the potential field is only a function of position, not velocity, Lagrange’s equations also follow directly from the equation of motion above:

\[ Q_j = \frac{d}{dt} \left( \frac{\partial (L + V)}{\partial \dot{q}_j} \right) - \frac{\partial (L + V)}{\partial q_j} = \left[ \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_j} \right) \right] + 0 \]

simplifying to

\[ \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_j} \right) = \frac{\partial L}{\partial q_j} \]

This is consistent with the results derived above and may be seen by differentiating the right side of the Lagrangian with respect to \( \dot{q}_j \) and time, and solely with respect to \( q_j \), adding the results and associating terms with the equations for \( F_i \) and \( Q_i \).

Newton’s laws

As the following derivation shows, no new physics is introduced, so the Lagrange equations can describe the dynamics of a classical system equivalently as Newton’s laws.

When \( q_i = r_i \) (i.e. the generalized coordinates are simply the Cartesian coordinates), it is straightforward to check that Lagrange’s equations reduce to Newton’s second law.

7.3.3 Dissipation function

In a more general formulation, the forces could be both potential and viscous. If an appropriate transformation can be found from the \( F_i \), Rayleigh suggests using a dissipation function, \( D \), of the following form:

\[ D = \frac{1}{2} \sum_{j=1}^{m} \sum_{k=1}^{m} C_{jk} \dot{q}_j \dot{q}_k \]

where \( C_{jk} \) are constants that are related to the damping coefficients in the physical system, though not necessarily equal to them.

If \( D \) is defined this way, then

\[ Q_j = - \frac{\partial V}{\partial q_j} - \frac{\partial D}{\partial \dot{q}_j} \]

and

\[ 0 = \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_j} \right) - \frac{\partial L}{\partial q_j} + \frac{\partial D}{\partial \dot{q}_j} \]

7.3.4 Examples

In this section two examples are provided in which the above concepts are applied. The first example establishes that in a simple case, the Newtonian approach and the Lagrangian formalism agree. The second case illustrates the power of the above formalism, in a case that is hard to solve with Newton’s laws.

Falling mass

Consider a point mass \( m \) falling freely from rest. By gravity a force \( F = mg \) is exerted on the mass (assuming \( g \) constant during the motion). Filling in the force in Newton’s law, we find \( \ddot{x} = g \) from which the solution

\[ x(t) = \frac{1}{2} gt^2 \]

follows (by taking the antiderivative of the antiderivative, and choosing the origin as the starting point). This result
can also be derived through the Lagrangian formalism. Take \( x \) to be the coordinate, which is \( \theta \) at the starting point. The kinetic energy is \( T = \frac{1}{2} m \dot{x}^2 \) and the potential energy is \( V = -mgx \); hence,
\[
L = T - V = \frac{1}{2} m \dot{x}^2 + mgx.
\]
Then
\[
0 = \frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} = mg - m \frac{d\dot{x}}{dt}
\]
which can be rewritten as \( \ddot{x} = g \), yielding the same result as earlier.

**Pendulum on a movable support**

Consider a pendulum of mass \( m \) and length \( \ell \), which is attached to a support with mass \( M \), which can move along a line in the \( x \)-direction. Let \( x \) be the coordinate along the line of the support, and let us denote the position of the pendulum by the angle \( \theta \) from the vertical.

![Sketch of the situation with definition of the coordinates](https://via.placeholder.com/150)

The kinetic energy can then be shown to be
\[
T = \frac{1}{2} M \dot{x}^2 + \frac{1}{2} m \left( \dot{\theta}^2 + \dot{\theta} \dot{x} \cos \theta \right)^2
\]
and the potential energy of the system is
\[
V = mg \dot{x} \cos \theta = -mg \theta.
\]
The Lagrangian is therefore
\[
L = T - V = \frac{1}{2} M \dot{x}^2 + \frac{1}{2} m \left[ \dot{\theta}^2 + \left( \ell \dot{x} \sin \theta \right)^2 \right] + m g \ell \cos \theta
\]
\[
= \frac{1}{2} (M + m) \dot{x}^2 + m \ell \dot{x} \dot{\theta} \cos \theta + \frac{1}{2} m \ell^2 \dot{\theta}^2 + m g \ell \cos \theta
\]
Now carrying out the differentiations gives for the support coordinate \( x \)
\[
\frac{d}{dt} \left[ (M + m) \dot{x} + m \ell \dot{\theta} \cos \theta \right] = 0,
\]
therefore:
\[
(M + m) \ddot{x} + m \ell \ddot{\theta} \cos \theta - m \ell \dot{\theta}^2 \sin \theta = 0
\]
indicating the presence of a constant of motion. Performing the same procedure for the variable \( \theta \) yields:
\[
\frac{d}{dt} \left[ m (\dot{x} \ell \cos \theta + \ell^2 \dot{\theta}) \right] + m \ell (\dot{x} \dot{\theta} + g) \sin \theta = 0;
\]
therefore
\[
\ddot{\theta} + \frac{\ddot{x}}{\ell} \cos \theta + \frac{g}{\ell} \sin \theta = 0.
\]
These equations may look quite complicated, but finding them with Newton’s laws would have required carefully identifying all forces, which would have been much more laborious and prone to errors. By considering limit cases, the correctness of this system can be verified: For example, \( \ddot{x} \to 0 \) should give the equations of motion for a pendulum that is at rest in some inertial frame, while \( \ddot{\theta} \to 0 \) should give the equations for a pendulum in a constantly accelerating system, etc. Furthermore, it is trivial to obtain the results numerically, given suitable starting conditions and a chosen time step, by stepping through the results iteratively.

**Two-body central force problem**

The basic problem is that of two bodies in orbit about each other attracted by a central force. The Jacobi coordinates are introduced; namely, the location of the center of mass \( \mathbf{R} \) and the separation of the bodies \( \mathbf{r} \) (the relative position). The Lagrangian is then
\[
L = T - U = \frac{1}{2} M \dot{\mathbf{R}}^2 + \frac{1}{2} \mu \dot{\mathbf{r}}^2 - U(\mathbf{r})
\]
\[
= L_{cm} + L_{rel}
\]
where \( M \) is the total mass, \( \mu \) is the reduced mass, and \( U \) the potential of the radial force. The Lagrangian is
7.4. EXTENSIONS OF LAGRANGIAN MECHANICS

divided into a center-of-mass term and a relative motion term. The $\textbf{R}$ equation from the Euler–Lagrange system is simply:

$$M \ddot{\textbf{R}} = 0,$$
resulting in simple motion of the center of mass in a straight line at constant velocity. The relative motion is expressed in polar coordinates $(r, \theta)$:

$$L = \frac{1}{2} \mu \left( \dot{r}^2 + r^2 \dot{\theta}^2 \right) - U(r),$$

which does not depend upon $\theta$, therefore an ignorable coordinate. The Lagrange equation for $\theta$ is then:

$$\frac{\partial L}{\partial \dot{\theta}} = \mu r^2 \ddot{\theta} = \text{constant} = \ell,$$

where $\ell$ is the conserved angular momentum. The Lagrange equation for $r$ is:

$$\frac{\partial L}{\partial r} = \frac{d}{dt} \frac{\partial L}{\partial \dot{r}},$$
or:

$$\mu r^2 \ddot{\theta} - \frac{dU}{dr} = \mu \ddot{r}.$$

This equation is identical to the radial equation obtained using Newton’s laws in a co-rotating reference frame, that is, a frame rotating with the reduced mass so it appears stationary. If the angular velocity is replaced by its value in terms of the angular momentum,

$$\dot{\theta} = \frac{\ell}{\mu r^2},$$

the radial equation becomes:[13]

$$\mu \ddot{r} = -\frac{dU}{dr} + \frac{\ell^2}{\mu r^3},$$

which is the equation of motion for a one-dimensional problem in which a particle of mass $\mu$ is subjected to the inward central force $-dU/dr$ and a second outward force, called in this context the centrifugal force:

$$F_{ct} = \mu \ddot{r} = \frac{\ell^2}{\mu r^3}.$$

Of course, if one remains entirely within the one-dimensional formulation, $\ell$ enters only as some imposed parameter of the external outward force, and its interpretation as angular momentum depends upon the more general two-dimensional problem from which the one-dimensional problem originated.

If one arrives at this equation using Newtonian mechanics in a co-rotating frame, the interpretation is evident as the centrifugal force in that frame due to the rotation of the frame itself. If one arrives at this equation directly by using the generalized coordinates $(r, \theta)$ and simply following the Lagrangian formulation without thinking about frames at all, the interpretation is that the centrifugal force is an outgrowth of using polar coordinates. As Hildebrand says:[14] “Since such quantities are not true physical forces, they are often called inertial forces. Their presence or absence depends, not upon the particular problem at hand, but upon the coordinate system chosen.” In particular, if Cartesian coordinates are chosen, the centrifugal force disappears, and the formulation involves only the central force itself, which provides the centripetal force for a curved motion.

This viewpoint, that fictitious forces originate in the choice of coordinates, often is expressed by users of the Lagrangian method. This view arises naturally in the Lagrangian approach, because the frame of reference is (possibly unconsciously) selected by the choice of coordinates.[15] Unfortunately, this usage of “inertial force” conflicts with the Newtonian idea of an inertial force. In the Newtonian view, an inertial force originates in the acceleration of the frame of observation (the fact that it is not an inertial frame of reference), not in the choice of coordinate system. To keep matters clear, it is safest to refer to the Lagrangian inertial forces as generalized inertial forces, to distinguish them from the Newtonian vector inertial forces. That is, one should avoid following Hildebrand when he says (p. 155) “we deal always with generalized forces, velocities accelerations, and momenta. For brevity, the adjective "generalized" will be omitted frequently.”

It is known that the Lagrangian of a system is not unique. Within the Lagrangian formalism the Newtonian fictitious forces can be identified by the existence of alternative Lagrangians in which the fictitious forces disappear, sometimes found by exploiting the symmetry of the system.[16]

7.4 Extensions of Lagrangian mechanics

The Hamiltonian, denoted by $H$, is obtained by performing a Legendre transformation on the Lagrangian, which introduces new variables, canonically conjugate to the original variables. This doubles the number of variables, but makes differential equations first order. The Hamiltonian is the basis for an alternative formulation of classical mechanics known as Hamiltonian mechanics. It is a par-
particularly ubiquitous quantity in quantum mechanics (see Hamiltonian (quantum mechanics)).

In 1948, Feynman discovered the path integral formulation extending the principle of least action to quantum mechanics for electrons and photons. In this formulation, particles travel every possible path between the initial and final states; the probability of a specific final state is obtained by summing over all possible trajectories leading to it. In the classical regime, the path integral formulation cleanly reproduces Hamilton’s principle, and Fermat’s principle in optics.

Dissipation (i.e. non-conservative systems) can also be treated with an effective Lagrangian formulated by a certain doubling of the degrees of freedom; see.[17][18][19][20]

7.5 See also

- Canonical coordinates
- Functional derivative
- Generalized coordinates
- Hamiltonian mechanics
- Hamiltonian optics
- Lagrangian analysis (applications of Lagrangian mechanics)
- Lagrangian point
- Non-autonomous mechanics
- Restricted three-body problem

7.6 References

[18] “Classical Mechanics of Nonconservative Systems” by Chad Galley
[19] “Radiation reaction at the level of the action” by Ofek Birnholtz, Shahar Hadar, and Barak Kol

7.7 Further reading

- Gupta, Kiran Chandra, Classical mechanics of particles and rigid bodies (Wiley, 1988).
- Goldstein, Herbert, Classical Mechanics, Addison Wesley.
7.8. **EXTERNAL LINKS**


### 7.8 External links

- Tong, David, Classical Dynamics Cambridge lecture notes
- Principle of least action interactive Excellent interactive explanation/webpage
- Joseph Louis de Lagrange - Œuvres complètes (Gallica-Math)
Chapter 8

Hamiltonian mechanics

Hamiltonian mechanics is a theory developed as a reformulation of classical mechanics and predicts the same outcomes as non-Hamiltonian classical mechanics. It uses a different mathematical formalism, providing a more abstract understanding of the theory. Historically, it was an important reformulation of classical mechanics, which later contributed to the formulation of quantum mechanics.

Hamiltonian mechanics was first formulated by William Rowan Hamilton in 1833, starting from Lagrangian mechanics, a previous reformulation of classical mechanics introduced by Joseph Louis Lagrange in 1788.

8.1 Overview

In Hamiltonian mechanics, a classical physical system is described by a set of canonical coordinates \( r = (q, p) \), where each component of the coordinate \( q_i \), \( p_i \) is indexed to the frame of reference of the system.

The time evolution of the system is uniquely defined by Hamilton’s equations:

\[ \frac{\partial H}{\partial q_i} = p_i, \quad \frac{\partial H}{\partial p_i} = \frac{\partial T}{\partial q_i} - \frac{\partial V}{\partial q_i}, \]

where \( H = H(q, p, t) \) is the Hamiltonian, which often corresponds to the total energy of the system.\(^{[3]}\) For a closed system, it is the sum of the kinetic and potential energy in the system.

In classical mechanics, the time evolution is obtained by computing the total force being exerted on each particle of the system, and from Newton’s second law, the time-evolutions of both position and velocity are computed. In contrast, in Hamiltonian mechanics, the time evolution is obtained by computing the Hamiltonian of the system in the generalized coordinates and inserting it in the Hamiltonian equations. It is important to point out that this approach is equivalent to the one used in Lagrangian mechanics. In fact, as will be shown below, the Hamiltonian is the Legendre transform of the Lagrangian, and thus both approaches give the same equations for the same generalized momentum. The main motivation to use Hamiltonian mechanics instead of Lagrangian mechanics comes from the symplectic structure of Hamiltonian systems.

While Hamiltonian mechanics can be used to describe simple systems such as a bouncing ball, a pendulum or an oscillating spring in which energy changes from kinetic to potential and back again over time, its strength is shown in more complex dynamic systems, such as planetary orbits in celestial mechanics.\(^{[3]}\) Naturally, the more degrees of freedom the system has, the more complicated its time evolution is and, in most cases, it becomes chaotic.

8.1.1 Basic physical interpretation

A simple interpretation of the Hamilton mechanics comes from its application on a one-dimensional system consisting of one particle of mass \( m \) under no external forces applied. The Hamiltonian represents the total energy of the system, which is the sum of kinetic and potential energy, traditionally denoted \( T \) and \( V \), respectively. Here \( q \) is the coordinate and \( p \) is the momentum, \( mv \). Then

\[ H = T + V, \quad T = \frac{p^2}{2m}, \quad V = V(q). \]

Note that \( T \) is a function of \( p \) alone, while \( V \) is a function of \( q \) alone (i.e., \( T \) and \( V \) are scleronomic).

In this example, the time-derivative of the momentum \( p \) equals the Newtonian force, and so the first Hamilton equation means that the force equals the negative gradient of potential energy. The time-derivative of \( q \) is the velocity, and so the second Hamilton equation means that the particle’s velocity equals the derivative of its kinetic energy with respect to its momentum.

8.1.2 Calculating a Hamiltonian from a Lagrangian

Given a Lagrangian in terms of the generalized coordinates \( q_i \) and generalized velocities \( \dot{q}_i \) and time:

1. The momenta are calculated by differentiating the
Lagrangian with respect to the (generalized) velocities: \( p_i(q_i, \dot{q}_i, t) = \frac{\partial L}{\partial \dot{q}_i} \).

2. The velocities \( \dot{q}_i \) are expressed in terms of the momenta \( p_i \) by inverting the expressions in the previous step.

3. The Hamiltonian is calculated using the usual definition of \( \mathcal{H} \) as the Legendre transformation of \( \mathcal{L} \) :
\[
\mathcal{H} = \sum_i \dot{q}_i \frac{\partial \mathcal{L}}{\partial \dot{q}_i} - \mathcal{L} = \sum_i \dot{q}_i p_i - \mathcal{L}.
\]
The velocities are substituted for using the previous results.

### 8.2 Deriving Hamilton’s equations

Hamilton’s equations can be derived by looking at how the total differential of the Lagrangian depends on time, generalized positions \( q_i \) and generalized velocities \( \dot{q}_i \) :

\[
d\mathcal{L} = \sum_i \left( \frac{\partial \mathcal{L}}{\partial q_i} dq_i + \frac{\partial \mathcal{L}}{\partial \dot{q}_i} d\dot{q}_i \right) + \frac{\partial \mathcal{L}}{\partial t} dt.
\]

Now the generalized momenta were defined as

\[
p_i = \frac{\partial \mathcal{L}}{\partial \dot{q}_i}.
\]
If this is substituted into the total differential of the Lagrangian, one gets

\[
d\mathcal{L} = \sum_i \left( \frac{\partial \mathcal{L}}{\partial q_i} dq_i + p_i d\dot{q}_i \right) + \frac{\partial \mathcal{L}}{\partial t} dt.
\]

We can rewrite this as

\[
d\mathcal{L} = \sum_i \left( \frac{\partial \mathcal{L}}{\partial q_i} dq_i + p_i d\dot{q}_i \right) + \frac{\partial \mathcal{L}}{\partial t} dt
\]

and rearrange again to get

\[
d \left( \sum_i p_i \dot{q}_i - \mathcal{L} \right) = \sum_i \left( \frac{\partial \mathcal{L}}{\partial q_i} dq_i + \dot{q}_i dp_i \right) - \frac{\partial \mathcal{L}}{\partial t} dt.
\]

The term on the left-hand side is just the Hamiltonian that we have defined before, so we find that

\[
d\mathcal{H} = \sum_i \left( -\frac{\partial \mathcal{L}}{\partial q_i} dq_i - \dot{q}_i dp_i \right) - \frac{\partial \mathcal{L}}{\partial t} dt.
\]

We can also calculate the total differential of the Hamiltonian \( \mathcal{H} \) with respect to time directly, as we did with the Lagrangian \( \mathcal{L} \) above, yielding:

\[
d\mathcal{H} = \sum_i \left( -\frac{\partial \mathcal{L}}{\partial q_i} dq_i - \dot{q}_i dp_i \right) - \frac{\partial \mathcal{L}}{\partial t} dt.
\]

It follows from the previous two independent equations that their right-hand sides are equal with each other. Thus we obtain the equation

\[
\sum_i \left( -\frac{\partial \mathcal{L}}{\partial q_i} dq_i + \dot{q}_i dp_i \right) - \frac{\partial \mathcal{L}}{\partial t} dt = \sum_i \left( \frac{\partial \mathcal{H}}{\partial q_i} dq_i + \frac{\partial \mathcal{H}}{\partial p_i} dp_i \right) + \frac{\partial \mathcal{H}}{\partial t} dt.
\]

Since this calculation was done off-shell, we can associate corresponding terms from both sides of this equation to yield:

\[
\frac{\partial \mathcal{H}}{\partial q_i} = -\frac{\partial \mathcal{L}}{\partial \dot{q}_i}, \quad \frac{\partial \mathcal{H}}{\partial p_i} = \dot{q}_i, \quad \frac{\partial \mathcal{H}}{\partial t} = -\frac{\partial \mathcal{L}}{\partial t}.
\]

On-shell, Lagrange’s equations tell us that

\[
\frac{\partial \mathcal{L}}{\partial \dot{q}_i} = \dot{p}_i.
\]

Thus Hamilton’s equations hold on-shell:

\[
\frac{\partial \mathcal{H}}{\partial q_j} = -\dot{p}_j, \quad \frac{\partial \mathcal{H}}{\partial p_j} = \dot{q}_j, \quad \frac{\partial \mathcal{H}}{\partial t} = -\frac{\partial \mathcal{L}}{\partial t}.
\]

### 8.3 As a reformulation of Lagrangian mechanics

Starting with Lagrangian mechanics, the equations of motion are based on generalized coordinates

\[
\{ q_j \mid j = 1, \ldots, N \}
\]

and matching generalized velocities

\[
\{ \dot{q}_j \mid j = 1, \ldots, N \}.
\]

We write the Lagrangian as

\[
\mathcal{L}(q_j, \dot{q}_j, t)
\]
with the subscripted variables understood to represent all $N$ variables of that type. Hamiltonian mechanics aims to replace the generalized velocity variables with generalized momentum variables, also known as conjugate momenta. By doing so, it is possible to handle certain systems, such as aspects of quantum mechanics, that would otherwise be even more complicated.

For each generalized velocity, there is one corresponding conjugate momentum, defined as:

$$p_j = \frac{\partial L}{\partial \dot{q}_j}.$$ 

In Cartesian coordinates, the generalized momenta are precisely the physical linear momenta. In circular polar coordinates, the generalized momentum corresponding to the angular velocity is the physical angular momentum. For an arbitrary choice of generalized coordinates, it may not be possible to obtain an intuitive interpretation of the conjugate momenta.

One thing which is not too obvious in this coordinate dependent formulation is that different generalized coordinates are really nothing more than different coordinate patches on the same symplectic manifold (see Mathematical formalism, below).

The Hamiltonian is the Legendre transform of the Lagrangian:

$$\mathcal{H}(q_j, p_j, t) = \sum_i \dot{q}_i p_i - \mathcal{L}(q_j, \dot{q}_j, t).$$

If the transformation equations defining the generalized coordinates are independent of $t$, and the Lagrangian is a sum of products of functions (in the generalized coordinates) which are homogeneous of order 0, 1 or 2, then it can be shown that $H$ is equal to the total energy $E = T + V$.

Each side in the definition of $\mathcal{H}$ produces a differential:

$$d\mathcal{H} = \sum_i \left[ \left( \frac{\partial \mathcal{H}}{\partial \dot{q}_i} \right) d\dot{q}_i + \left( \frac{\partial \mathcal{H}}{\partial p_i} \right) dp_i + \frac{\partial \mathcal{H}}{\partial t} dt \right]$$

$$= \sum_i \left[ \dot{q}_i dp_i + p_i d\dot{q}_i - \left( \frac{\partial \mathcal{L}}{\partial q_i} \right) dq_i - \left( \frac{\partial \mathcal{L}}{\partial \dot{q}_i} \right) d\dot{q}_i \right]$$

Substituting the previous definition of the conjugate momenta into this equation and matching coefficients, we obtain the equations of motion of Hamiltonian mechanics, known as the canonical equations of Hamilton:

$$\frac{\partial \mathcal{H}}{\partial \dot{q}_j} = -\dot{p}_j, \quad \frac{\partial \mathcal{H}}{\partial p_j} = \dot{q}_j, \quad \frac{\partial \mathcal{H}}{\partial t} = -\frac{\partial \mathcal{L}}{\partial t}.$$ 

Hamilton’s equations consist of 2n first-order differential equations, while Lagrange’s equations consist of n second-order equations. However, Hamilton’s equations usually don’t reduce the difficulty of finding explicit solutions. They still offer some advantages, since important theoretical results can be derived because coordinates and momenta are independent variables with nearly symmetric roles.

Hamilton’s equations have another advantage over Lagrange’s equations: if a system has a symmetry, such that a coordinate does not occur in the Hamiltonian, the corresponding momentum is conserved, and that coordinate can be ignored in the other equations of the set. Effectively, this reduces the problem from n coordinates to (n-1) coordinates. In the Lagrangian framework, of course the result that the corresponding momentum is conserved still follows immediately, but all the generalized velocities still occur in the Lagrangian - we still have to solve a system of equations in n coordinates.[2]

The Lagrangian and Hamiltonian approaches provide the groundwork for deeper results in the theory of classical mechanics, and for formulations of quantum mechanics.

### 8.4 Geometry of Hamiltonian systems

A Hamiltonian system may be understood as a fiber bundle $E$ over time $R$, with the fibers $E_t$, $t \in R$, being the position space. The Lagrangian is thus a function on the jet bundle $J$ over $E$; taking the fiberwise Legendre transform of the Lagrangian produces a function on the dual bundle over time whose fiber at $t$ is the cotangent space $T^*E_t$, which comes equipped with a natural symplectic form, and this latter function is the Hamiltonian.

### 8.5 Generalization to quantum mechanics through Poisson bracket

Hamilton’s equations above work well for classical mechanics, but not for quantum mechanics, since the differential equations discussed assume that one can specify the exact position and momentum of the particle simultaneously at any point in time. However, the equations can be further generalized to then be extended to apply to quantum mechanics as well as to classical mechanics, through the deformation of the Poisson algebra over $p$ and $q$ to the algebra of Moyal brackets.

Specifically, the more general form of the Hamilton’s equation reads
\[
\frac{df}{dt} = \{ f, \mathcal{H} \} + \frac{\partial f}{\partial t}.
\]

where \( f \) is some function of \( p \) and \( q \), and \( \mathcal{H} \) is the Hamiltonian. To find out the rules for evaluating a Poisson bracket without resorting to differential equations, see Lie algebra; a Poisson bracket is the name for the Lie bracket in a Poisson algebra. These Poisson brackets can then be extended to Moyal brackets comporting to an inequivalent Lie algebra, as proven by H. Groenewold, and thereby describe quantum mechanical diffusion in phase space (See the phase space formulation and Weyl quantization). This more algebraic approach not only permits ultimately extending probability distributions in phase space to Wigner quasi-probability distributions, but, at the mere Poisson bracket classical setting, also provides more power in helping analyze the relevant conserved quantities in a system.

### 8.6 Mathematical formalism

Any smooth real-valued function \( H \) on a symplectic manifold can be used to define a Hamiltonian system. The function \( H \) is known as the Hamiltonian or the energy function. The symplectic manifold is then called the phase space. The Hamiltonian induces a special vector field on the symplectic manifold, known as the Hamiltonian vector field.

The Hamiltonian vector field (a special type of symplectic vector field) induces a Hamiltonian flow on the manifold. This is a one-parameter family of transformations of the manifold (the parameter of the curves is commonly called the time); in other words an isotopy of symplectomorphisms, starting with the identity. By Liouville’s theorem, each symplectomorphism preserves the volume form on the phase space. The collection of symplectomorphisms induced by the Hamiltonian flow is commonly called the Hamiltonian mechanics of the Hamiltonian system.

The symplectic structure induces a Poisson bracket. The Poisson bracket gives the space of functions on the manifold the structure of a Lie algebra.

Given a function \( f \)

\[
\frac{d}{dt} f = \frac{\partial}{\partial t} f + \{ f, \mathcal{H} \}.
\]

If we have a probability distribution, \( \rho \), then (since the phase space velocity \( \langle \dot{\rho}, \dot{\mathcal{H}} \rangle \) has zero divergence, and probability is conserved) its convective derivative can be shown to be zero and so

\[
\frac{\partial}{\partial t} \rho = -\{ \rho, \mathcal{H} \}.
\]

This is called Liouville’s theorem. Every smooth function \( G \) over the symplectic manifold generates a one-parameter family of symplectomorphisms and if \( \{ G, H \} = 0 \), then \( G \) is conserved and the symplectomorphisms are symmetry transformations.

A Hamiltonian may have multiple conserved quantities \( G_i \). If the symplectic manifold has dimension \( 2n \) and there are \( n \) functionally independent conserved quantities \( G_i \) which are in involution (i.e., \( \{ G_i, G_j \} = 0 \)), then the Hamiltonian is Liouville integrable. The Liouville-Arnold theorem says that locally, any Liouville integrable Hamiltonian can be transformed via a symplectomorphism in a new Hamiltonian with the conserved quantities \( G_i \) as coordinates; the new coordinates are called action-angle coordinates. The transformed Hamiltonian depends only on the \( G_i \), and hence the equations of motion have the simple form

\[
\dot{G}_i = 0, \quad \varphi_i = F(G),
\]

for some function \( F \) (Arnol’d et al., 1988). There is an entire field focusing on small deviations from integrable systems governed by the KAM theorem.

The integrability of Hamiltonian vector fields is an open question. In general, Hamiltonian systems are chaotic; concepts of measure, completeness, integrability and stability are poorly defined. At this time, the study of dynamical systems is primarily qualitative, and not a quantitative science.

### 8.7 Riemannian manifolds

An important special case consists of those Hamiltonians that are quadratic forms, that is, Hamiltonians that can be written as

\[
\mathcal{H}(q, p) = \frac{1}{2} \langle p, p \rangle_q
\]

where \( \langle \cdot, \cdot \rangle_q \) is a smoothly varying inner product on the fibers \( T^*_q Q \), the cotangent space to the point \( q \) in the configuration space, sometimes called a cometric. This Hamiltonian consists entirely of the kinetic term.

If one considers a Riemannian manifold or a pseudo-Riemannian manifold, the Riemannian metric induces a linear isomorphism between the tangent and cotangent bundles. (See Musical isomorphism). Using this isomorphism, one can define a cometric. (In coordinates, the matrix defining the cometric is the inverse of the matrix defining the metric.) The solutions to the Hamilton–Jacobi equations for this Hamiltonian are then the same as the geodesics on the manifold. In particular, the Hamiltonian flow in this case is the same thing as the geodesic flow. The existence of such solutions, and the
completeness of the set of solutions, are discussed in detail in the article on geodesics. See also Geodesics as Hamiltonian flows.

8.8 Sub-Riemannian manifolds

When the cometric is degenerate, then it is not invertible. In this case, one does not have a Riemannian manifold, as one does not have a metric. However, the Hamiltonian still exists. In the case where the cometric is degenerate at every point \( q \) of the configuration space manifold \( Q \), so that the rank of the cometric is less than the dimension of the manifold \( Q \), one has a sub-Riemannian manifold.

The Hamiltonian in this case is known as a sub-Riemannian Hamiltonian. Every such Hamiltonian uniquely determines the cometric, and vice-versa. This implies that every sub-Riemannian manifold is uniquely determined by its sub-Riemannian Hamiltonian, and that the converse is true: every sub-Riemannian manifold has a unique sub-Riemannian Hamiltonian. The existence of sub-Riemannian geodesics is given by the Chow–Rashevskii theorem.

The continuous, real-valued Heisenberg group provides a simple example of a sub-Riemannian manifold. For the Heisenberg group, the Hamiltonian is given by

\[
\mathcal{H}(x, y, z, p_x, p_y, p_z) = \frac{1}{2} \left( p_x^2 + p_y^2 \right).
\]

\( p_z \) is not involved in the Hamiltonian.

8.9 Poisson algebras

Hamiltonian systems can be generalized in various ways. Instead of simply looking at the algebra of smooth functions over a symplectic manifold, Hamiltonian mechanics can be formulated on general commutative unital real Poisson algebras. A state is a continuous linear functional on the Poisson algebra (equipped with some suitable topology) such that for any element \( A \) of the algebra, \( A^2 \) maps to a nonnegative real number.

A further generalization is given by Nambu dynamics.

8.10 Charged particle in an electromagnetic field

A good illustration of Hamiltonian mechanics is given by the Hamiltonian of a charged particle in an electromagnetic field. In Cartesian coordinates (i.e. \( q_i = x_i \)), the Lagrangian of a non-relativistic classical particle in an electromagnetic field is (in SI Units):

\[
\mathcal{L} = \sum_i \frac{1}{2} m \dot{x}_i^2 + \sum_i e \dot{x}_i A_i - e\phi,
\]

where \( e \) is the electric charge of the particle (not necessarily the elementary charge), \( \phi \) is the electric scalar potential, and the \( A_i \) are the components of the magnetic vector potential (these may be modified through a gauge transformation). This is called minimal coupling.

The generalized momenta are given by:

\[
p_i = \frac{\partial \mathcal{L}}{\partial \dot{x}_i} = m \dot{x}_i + e A_i.
\]

Rearranging, the velocities are expressed in terms of the momenta:

\[
\dot{x}_i = \frac{p_i - e A_i}{m}.
\]

If we substitute the definition of the momenta, and the definitions of the velocities in terms of the momenta, into the definition of the Hamiltonian given above, and then simplify and rearrange, we get:

\[
\mathcal{H} = \sum_i \dot{x}_i p_i - \mathcal{L} = \sum_i \frac{(p_i - e A_i)^2}{2m} + e\phi.
\]

This equation is used frequently in quantum mechanics.

8.11 Relativistic charged particle in an electromagnetic field

The Lagrangian for a relativistic charged particle is given by:

\[
\mathcal{L}(t) = -mc^2 \sqrt{1 - \frac{\vec{\dot{x}}(t)^2}{c^2}} - e\phi(\vec{x}(t), t) + e\vec{x}(t) \cdot \vec{A}(\vec{x}(t), t).
\]

Thus the particle’s canonical (total) momentum is

\[
\vec{P}(t) = \frac{\partial \mathcal{L}(t)}{\partial \dot{x}(t)} = \frac{m \vec{\dot{x}}(t)}{\sqrt{1 - \frac{\vec{\dot{x}}(t)^2}{c^2}}} + e\vec{A}(\vec{x}(t), t),
\]

that is, the sum of the kinetic momentum and the potential momentum.

Solving for the velocity, we get

\[
\dot{x}(t) = \frac{\vec{P}(t) - e\vec{A}(\vec{x}(t), t)}{\sqrt{m^2 + \frac{1}{c^2} \left( \vec{P}(t) - e\vec{A}(\vec{x}(t), t) \right)^2}}.
\]
8.13 References

8.13.1 Footnotes


[4] This derivation is along the lines as given in Arnol'd 1989, pp. 65–66

8.13.2 Sources


8.14 External links

- Binney, James J., Classical Mechanics (lecture notes), University of Oxford, retrieved 27 October 2010

- Tong, David, Classical Dynamics (Cambridge lecture notes), University of Cambridge, retrieved 27 October 2010

- Hamilton, William Rowan, On a General Method in Dynamics, Trinity College Dublin
Chapter 9

Classical mechanics

Diagram of orbital motion of a satellite around the earth, showing perpendicular velocity and acceleration (force) vectors.

In physics, classical mechanics and quantum mechanics are the two major sub-fields of mechanics. Classical mechanics is concerned with the set of physical laws describing the motion of bodies under the action of a system of forces. The study of the motion of bodies is an ancient one, making classical mechanics one of the oldest and largest subjects in science, engineering and technology. It is also widely known as Newtonian mechanics.

Classical mechanics describes the motion of macroscopic objects, from projectiles to parts of machinery, as well as astronomical objects, such as spacecraft, planets, stars, and galaxies. Besides this, many specializations within the subject deal with solids, liquids and gases and other specific sub-topics. Classical mechanics also provides extremely accurate results as long as the domain of study is restricted to large objects and the speeds involved do not approach the speed of light. When the objects being dealt with become sufficiently small, it becomes necessary to introduce the other major sub-field of mechanics, quantum mechanics, which reconciles the macroscopic laws of physics with the atomic nature of matter and handles the wave–particle duality of atoms and molecules. However, when both quantum mechanics and classical mechanics cannot apply, such as at the quantum level with many degrees of freedom, quantum field theory (QFT) becomes applicable. QFT deals with small distances and large speeds with many degrees of freedom as well as the possibility of any change in the number of particles throughout the interaction. To deal with large degrees of freedom at the macroscopic level, statistical mechanics becomes valid. Statistical mechanics explores the large number of particles and their interactions as a whole in everyday life. Statistical mechanics is mainly used in thermodynamics. In the case of high velocity objects approaching the speed of light, classical mechanics is enhanced by special relativity. General relativity unifies special relativity with Newton’s law of universal gravitation, allowing physicists to handle gravitation at a deeper level.

The term classical mechanics was coined in the early 20th century to describe the system of physics begun by Isaac Newton and many contemporary 17th century natural philosophers, building upon the earlier astronomical theories of Johannes Kepler, which in turn were based on the precise observations of Tycho Brahe and the studies of terrestrial projectile motion of Galileo. Since these aspects of physics were developed long before the emergence of quantum physics and relativity, some sources exclude Einstein’s theory of relativity from this category. However, a number of modern sources do include relativistic mechanics, which in their view represents classical mechanics in its most developed and most accurate form.[note 1]

The initial stage in the development of classical mechanics is often referred to as Newtonian mechanics, and is associated with the physical concepts employed by and the mathematical methods invented by Newton himself, in parallel with Leibniz, and others. This is further described in the following sections. Later, more abstract and general methods were developed, leading to reformulations of classical mechanics known as Lagrangian mechanics and Hamiltonian mechanics. These advances were largely made in the 18th and 19th centuries, and they extend substantially beyond Newton’s work, particularly through their use of analytical mechanics. Ultimately, the mathematics developed for these were central to the creation of quantum mechanics.
9.1 History

Main article: History of classical mechanics
See also: Timeline of classical mechanics

Some Greek philosophers of antiquity, among them Aristotle, founder of Aristotelian physics, may have been the first to maintain the idea that “everything happens for a reason” and that theoretical principles can assist in the understanding of nature. While to a modern reader, many of these preserved ideas come forth as eminently reasonable, there is a conspicuous lack of both mathematical theory and controlled experiment, as we know it. These both turned out to be decisive factors in forming modern science, and they started out with classical mechanics.

In his *Elementa super demonstrationem ponderum*, medieval mathematician Jordanus de Nemore concept of "positional gravity" and the use of component forces.

As foundation for his principles of natural philosophy, Isaac Newton proposed three laws of motion: the law of inertia, his second law of acceleration (mentioned above), and the law of action and reaction; and hence laid the foundations for classical mechanics. Both Newton’s second and third laws were given proper scientific and mathematical treatment in Newton’s *Philosophiae Naturalis Principia Mathematica*, which distinguishes them from earlier attempts at explaining similar phenomena, which were either incomplete, incorrect, or given little accurate mathematical expression. Newton also enunciated the principles of conservation of momentum and angular momentum. In mechanics, Newton was also the first to provide the first correct scientific and mathematical formulation of gravity in Newton’s law of universal gravitation. The combination of Newton’s laws of motion and gravitation provide the fullest and most accurate description of classical mechanics. He demonstrated that these laws apply to everyday objects as well as to celestial objects. In particular, he obtained a theoretical explanation of Kepler’s laws of motion of the planets.

Newton previously invented the calculus, of mathematics, and used it to perform the mathematical calculations. For acceptability, his book, the *Principia*, was formulated entirely in terms of the long-established geometric methods, which were soon eclipsed by his calculus. However, it was Leibniz who developed the notation of the *derivative* and *integral* preferred today.

Newton, and most of his contemporaries, with the notable exception of Huygens, worked on the assumption that classical mechanics would be able to explain all phenom-
Hamilton’s greatest contribution is perhaps the reformulation of Newtonian mechanics, now called Hamiltonian mechanics. Lagrangean mechanics was in turn re-formulated in 1833 by William Rowan Hamilton. Some difficulties were discovered in the late 19th century that could only be resolved by more modern physics. Some of these difficulties related to compatibility with electromagnetic theory, and the famous Michelson–Morley experiment. The resolution of these problems led to the special theory of relativity, often included in the term classical mechanics.

A second set of difficulties were related to thermodynamics. When combined with thermodynamics, classical mechanics leads to the Gibbs paradox of classical statistical mechanics, in which entropy is not a well-defined quantity. Black-body radiation was not explained without the introduction of quanta. As experiments reached the atomic level, classical mechanics failed to explain, even approximately, such basic things as the energy levels and sizes of atoms and the photo-electric effect. The effort at resolving these problems led to the development of quantum mechanics.

Since the end of the 20th century, the place of classical mechanics in physics has been no longer that of an independent theory. Instead, classical mechanics is now considered an approximate theory to the more general quantum mechanics. Emphasis has shifted to understanding the fundamental forces of nature as in the Standard model and its more modern extensions into a unified theory of everything. Classical mechanics is a theory for the study of the motion of non-quantum mechanical, low-energy particles in weak gravitational fields. In the 21st century classical mechanics has been extended into the complex domain and complex classical mechanics exhibits behaviors very similar to quantum mechanics.

9.2 Description of the theory

The analysis of projectile motion is a part of classical mechanics.

The following introduces the basic concepts of classical mechanics. For simplicity, it often models real-world objects as point particles, objects with negligible size. The motion of a point particle is characterized by a small number of parameters: its position, mass, and the forces applied to it. Each of these parameters is discussed in turn.

In reality, the kind of objects that classical mechanics can describe always have a non-zero size. (The physics of very small particles, such as the electron, is more accurately described by quantum mechanics.) Objects with non-zero size have more complicated behavior than hypothetical point particles, because of the additional degrees of freedom: a baseball can spin while it is moving, for example. However, the results for point particles can be used to study such objects by treating them as composite objects, made up of a large number of interacting point particles. The center of mass of a composite object behaves like a point particle.

Classical mechanics uses common-sense notions of how matter and forces exist and interact. It assumes that matter and energy have definite, knowable attributes
9.2. DESCRIPTION OF THE THEORY

such as where an object is in space and its speed. It also assumes that objects may be directly influenced only by their immediate surroundings, known as the principle of locality. In quantum mechanics, an object may have either its position or velocity undetermined.

9.2.1 Position and its derivatives

Main article: Kinematics

The position of a point particle is defined with respect to an arbitrary fixed reference point, O, in space, usually accompanied by a coordinate system, with the reference point located at the origin of the coordinate system. It is defined as the vector \( \mathbf{r} \) from O to the particle. In general, the point particle need not be stationary relative to O, so \( \mathbf{r} \) is a function of \( t \), the time elapsed since an arbitrary initial time. In pre-Einstein relativity (known as Galilean relativity), time is considered an absolute, i.e., the time interval between any given pair of events is the same for all observers.\(^4\) In addition to relying on absolute time, classical mechanics assumes Euclidean geometry for the structure of space.\(^5\)

Velocity and speed

Main articles: Velocity and speed

The velocity, or the rate of change of position with time, is defined as the derivative of the position with respect to time:

\[
\mathbf{v} = \frac{d\mathbf{r}}{dt}
\]

In classical mechanics, velocities are directly additive and subtractive. For example, if one car traveling east at 60 km/h passes another car traveling east at 50 km/h, then from the perspective of the slower car, the faster car is traveling east at \( 60 - 50 = 10 \) km/h. Whereas, from the perspective of the faster car, the slower car is moving 10 km/h to the west. Velocities are directly additive as vector quantities; they must be dealt with using vector analysis.

Mathematically, if the velocity of the first object in the previous discussion is denoted by the vector \( \mathbf{u} = \mathbf{v}d \) and the velocity of the second object by the vector \( \mathbf{v} = \mathbf{ve} \), where \( \mathbf{u} \) is the speed of the first object, \( \mathbf{v} \) is the speed of the second object, and \( \mathbf{d} \) and \( \mathbf{e} \) are unit vectors in the directions of motion of each particle respectively, then the velocity of the first object as seen by the second object is

\[
\mathbf{u}' = \mathbf{u} - \mathbf{v}.
\]

Similarly,

\[
\mathbf{v}' = \mathbf{v} - \mathbf{u}.
\]

When both objects are moving in the same direction, this equation can be simplified to

\[
\mathbf{u}' = (\mathbf{u} - \mathbf{v})d.
\]

Or, by ignoring direction, the difference can be given in terms of speed only:

\[
\mathbf{u}' = \mathbf{u} - \mathbf{v}.
\]

Acceleration

Main article: Acceleration

The acceleration, or rate of change of velocity, is the derivative of the velocity with respect to time (the second derivative of the position with respect to time):

\[
\mathbf{a} = \frac{d\mathbf{v}}{dt} = \frac{d^2\mathbf{r}}{dt^2}.
\]

Acceleration represents the velocity’s change over time: either of the velocity’s magnitude or direction, or both. If only the magnitude \( \mathbf{v} \) of the velocity decreases, this is sometimes referred to as deceleration, but generally any change in the velocity with time, including deceleration, is simply referred to as acceleration.

Frames of reference

Main articles: Inertial frame of reference and Galilean transformation

While the position, velocity and acceleration of a particle can be referred to any observer in any state of motion, classical mechanics assumes the existence of a special family of reference frames in terms of which the mechanical laws of nature take a comparatively simple form. These special reference frames are called inertial frames. An inertial frame is such that when an object without any force interactions (an idealized situation) is viewed from it, it appears either to be at rest or in a state of uniform motion in a straight line. This is the fundamental definition of an inertial frame. They are characterized by the requirement that all forces entering the observer’s physical laws originate in identifiable sources (charges, gravitational bodies, and so forth). A non-inertial reference frame is one accelerating with respect to an inertial one, and in such a non-inertial frame a particle is subject to acceleration by fictitious forces that enter the equations...
of motion solely as a result of its accelerated motion, and do not originate in identifiable sources. These fictitious forces are in addition to the real forces recognized in an inertial frame. A key concept of inertial frames is the method for identifying them. For practical purposes, reference frames that are unaccelerated with respect to the distant stars (an extremely distant point) are regarded as good approximations to inertial frames.

Consider two reference frames $S$ and $S'$. For observers in each of the reference frames an event has space-time coordinates of $(x,y,z,t)$ in frame $S$ and $(x',y',z',t')$ in frame $S'$. Assuming time is measured the same in all reference frames, and if we require $x = x'$ when $t = 0$, then the relation between the space-time coordinates of the same event observed from the reference frames $S'$ and $S$, which are moving at a relative velocity of $u$ in the $x$ direction is:

$$
x' = x - u t \\
y' = y \\
z' = z \\
t' = t.
$$

This set of formulas defines a group transformation known as the Galilean transformation (informally, the Galilean transform). This group is a limiting case of the Poincaré group used in special relativity. The limiting case applies when the velocity $u$ is very small compared to $c$, the speed of light.

The transformations have the following consequences:

- $v' = v - u$ (the velocity $v'$ of a particle from the perspective of $S'$ is slower by $u$ than its velocity $v$ from the perspective of $S$)
- $a' = a$ (the acceleration of a particle is the same in any inertial reference frame)
- $F' = F$ (the force on a particle is the same in any inertial reference frame)
- The speed of light is not a constant in classical mechanics, nor does the special position given to the speed of light in relativistic mechanics have a counterpart in classical mechanics.

For some problems, it is convenient to use rotating coordinates (reference frames). Thereby one can either keep a mapping to a convenient inertial frame, or introduce additionally a fictitious centrifugal force and Coriolis force.

### 9.2.2 Forces; Newton’s second law

Main articles: Force and Newton’s laws of motion

Newton was the first to mathematically express the relationship between force and momentum. Some physicists interpret Newton’s second law of motion as a definition of force and mass, while others consider it a fundamental postulate, a law of nature. Either interpretation has the same mathematical consequences, historically known as “Newton’s Second Law”:

$$F = \frac{dp}{dt} = \frac{d(mv)}{dt}.$$ 

The quantity $mv$ is called the (canonical) momentum. The net force on a particle is thus equal to the rate of change of the momentum of the particle with time. Since the definition of acceleration is $a = \frac{dv}{dt}$, the second law can be written in the simplified and more familiar form:

$$F = ma.$$ 

So long as the force acting on a particle is known, Newton’s second law is sufficient to describe the motion of a particle. Once independent relations for each force acting on a particle are available, they can be substituted into Newton’s second law to obtain an ordinary differential equation, which is called the equation of motion.

As an example, assume that friction is the only force acting on the particle, and that it may be modeled as a function of the velocity of the particle, for example:

$$F_R = -\lambda v,$$

where $\lambda$ is a positive constant. Then the equation of motion is

$$-\lambda v = ma = m \frac{dv}{dt}.$$ 

This can be integrated to obtain

$$v = v_0 e^{-\lambda t/m}$$

where $v_0$ is the initial velocity. This means that the velocity of this particle decays exponentially to zero as time progresses. In this case, an equivalent viewpoint is that the kinetic energy of the particle is absorbed by friction (which converts it to heat energy in accordance with the conservation of energy), and the particle is slowing down. This expression can be further integrated to obtain the position $r$ of the particle as a function of time.

Important forces include the gravitational force and the Lorenz force for electromagnetism. In addition, Newton’s third law can sometimes be used to deduce the forces acting on a particle: if it is known that particle A exerts a force $F$ on another particle B, it follows that B must exert an equal and opposite reaction force, $-F$, on A. The strong form of Newton’s third law requires that $F$ and $-F$ act along the line connecting A and B, while the weak form does not. Illustrations of the weak form of Newton’s third law are often found for magnetic forces.
9.2.3 Work and energy

Main articles: Work (physics), kinetic energy and potential energy

If a constant force $F$ is applied to a particle that achieves a displacement $\Delta r$, the work done by the force is defined as the scalar product of the force and displacement vectors:

$$W = F \cdot \Delta r.$$ 

More generally, if the force varies as a function of position as the particle moves from $r_1$ to $r_2$ along a path $C$, the work done on the particle is given by the line integral

$$W = \int_C F(r) \cdot dr.$$ 

If the work done in moving the particle from $r_1$ to $r_2$ is the same no matter what path is taken, the force is said to be conservative. Gravity is a conservative force, as is the force due to an idealized spring, as given by Hooke's law. The force due to friction is non-conservative.

The kinetic energy $E_k$ of a particle of mass $m$ travelling at speed $v$ is given by

$$E_k = \frac{1}{2} mv^2.$$ 

For extended objects composed of many particles, the kinetic energy of the composite body is the sum of the kinetic energies of the particles.

The work–energy theorem states that for a particle of constant mass $m$ the total work $W$ done on the particle from position $r_1$ to $r_2$ is equal to the change in kinetic energy $E_k$ of the particle:

$$W = \Delta E_k = E_{k,2} - E_{k,1} = \frac{1}{2} m \left( v^2 - v_1^2 \right).$$ 

Conservative forces can be expressed as the gradient of a scalar function, known as the potential energy and denoted $E_p$:

$$F = -\nabla E_p.$$ 

If all the forces acting on a particle are conservative, and $E_p$ is the total potential energy (which is defined as a work of involved forces to rearrange mutual positions of bodies), obtained by summing the potential energies corresponding to each force

$$F \cdot \Delta r = -\nabla E_p \cdot \Delta r = -\Delta E_p = -\Delta E_p = \Delta (E_k),$$

This result is known as conservation of energy and states that the total energy,

$$\sum E = E_k + E_p,$$

is constant in time. It is often useful, because many commonly encountered forces are conservative.

9.2.4 Beyond Newton’s laws

Classical mechanics also includes descriptions of the complex motions of extended non-pointlike objects. Euler's laws provide extensions to Newton's laws in this area. The concepts of angular momentum rely on the same calculus used to describe one-dimensional motion. The rocket equation extends the notion of rate of change of an object's momentum to include the effects of an object "losing mass".

There are two important alternative formulations of classical mechanics: Lagrangian mechanics and Hamiltonian mechanics. These, and other modern formulations, usually bypass the concept of “force”, instead referring to other physical quantities, such as energy, speed and momentum, for describing mechanical systems in generalized coordinates.

The expressions given above for momentum and kinetic energy are only valid when there is no significant electromagnetic contribution. In electromagnetism, Newton's second law for current-carrying wires breaks down unless one includes the electromagnetic field contribution to the momentum of the system as expressed by the Poynting vector divided by $c^2$, where $c$ is the speed of light in free space.

9.3 Limits of validity

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CHAPTER 9. CLASSICAL MECHANICS

Geometric optics is an approximation to the quantum theory of light, and does not have a superior “classical” form.

9.3.1 The Newtonian approximation to special relativity

In special relativity, the momentum of a particle is given by

\[ p = \frac{mv}{\sqrt{1 - (v^2/c^2)}} \]

where \( m \) is the particle’s rest mass, \( v \) its velocity, and \( c \) is the speed of light.

If \( v \) is very small compared to \( c \), \( v^2/c^2 \) is approximately zero, and so

\[ p \approx mv \]

Thus the Newtonian equation \( p = mv \) is an approximation of the relativistic equation for bodies moving with low speeds compared to the speed of light.

For example, the relativistic cyclotron frequency of a cyclotron, gyrotron, or high voltage magnetron is given by

\[ f = f_c \frac{m_0}{m_0 + T/c^2} \]

where \( f_c \) is the classical frequency of an electron (or other charged particle) with kinetic energy \( T \) and (rest) mass \( m_0 \) circling in a magnetic field. The (rest) mass of an electron is 511 keV. So the frequency correction is 1% for a magnetic vacuum tube with a 5.11 kV direct current accelerating voltage.

9.3.2 The classical approximation to quantum mechanics

The ray approximation of classical mechanics breaks down when the de Broglie wavelength is not much smaller than other dimensions of the system. For non-relativistic particles, this wavelength is

\[ \lambda = \frac{h}{p} \]

where \( h \) is Planck’s constant and \( p \) is the momentum.

Again, this happens with electrons before it happens with heavier particles. For example, the electrons used by Clinton Davisson and Lester Germer in 1927, accelerated by 54 volts, had a wavelength of 0.167 nm, which was long enough to exhibit a single diffraction side lobe when reflecting from the face of a nickel crystal with atomic spacing of 0.215 nm. With a larger vacuum chamber, it would seem relatively easy to increase the angular resolution from around a radian to a milliradian and see quantum diffraction from the periodic patterns of integrated circuit computer memory.

More practical examples of the failure of classical mechanics on an engineering scale are conduction by quantum tunneling in tunnel diodes and very narrow transistor gates in integrated circuits.

Classical mechanics is the same extreme high frequency approximation as geometric optics. It is more often accurate because it describes particles and bodies with rest mass. These have more momentum and therefore shorter de Broglie wavelengths than massless particles, such as light, with the same kinetic energies.

9.4 Branches

Classical mechanics was traditionally divided into three main branches:

- Statics, the study of equilibrium and its relation to forces
- Dynamics, the study of motion and its relation to forces
- Kinematics, dealing with the implications of observed motions without regard for circumstances causing them

Another division is based on the choice of mathematical formalism:

- Newtonian mechanics
- Lagrangian mechanics
- Hamiltonian mechanics

Alternatively, a division can be made by region of application:

- Celestial mechanics, relating to stars, planets and other celestial bodies
- Continuum mechanics, for materials modelled as a continuum, e.g., solids and fluids (i.e., liquids and gases).
- Relativistic mechanics (i.e., including the special and general theories of relativity), for bodies whose speed is close to the speed of light.
• Statistical mechanics, which provides a framework for relating the microscopic properties of individual atoms and molecules to the macroscopic or bulk thermodynamic properties of materials.

9.5 See also

• Dynamical systems
• History of classical mechanics
• List of equations in classical mechanics
• List of publications in classical mechanics
• Molecular dynamics
• Newton’s laws of motion
• Special theory of relativity

9.6 Notes

[1] The notion of “classical” may be somewhat confusing, insofar as this term usually refers to the era of classical antiquity in European history. While many discoveries within the mathematics of that period remain in full force today, and of the greatest use, much of the science that emerged then has since been superseded by more accurate models. This in no way detracts from the science of that time, though as most of modern physics is built directly upon the important developments, especially within technology, which took place in antiquity and during the Middle Ages in Europe and elsewhere. However, the emergence of classical mechanics was a decisive stage in the development of science, in the modern sense of the term. What characterizes it, above all, is its insistence on mathematics (rather than speculation), and its reliance on experiment (rather than observation). With classical mechanics it was established how to formulate quantitative predictions in theory, and how to test them by carefully designed measurement. The emerging globally cooperative endeavor increasingly provided for much closer scrutiny and testing, both of theory and experiment. This was, and remains, a key factor in establishing certain knowledge, and in bringing it to the service of society. History shows how closely the health and wealth of a society depends on nurturing this investigative and critical approach.

[2] The displacement \( \Delta r \) is the difference of the particle’s initial and final positions: \( \Delta r = r_f - r_i \).

9.7 References


[2] Page 2-10 of the Feynman Lectures on Physics says “For already in classical mechanics there was indeterminability from a practical point of view.” The past tense here implies that classical physics is no longer fundamental.

[3] Complex Elliptic Pendulum, Carl M. Bender, Daniel W. Hook, Karta Kooner


[5] MIT physics 8.01 lecture notes (page 12) (PDF)

9.8 Further reading


• M. Alonso; J. Finn. Fundamental university physics. Addison-Wesley.


9.9 External links

- Crowell, Benjamin. *Newtonian Physics* (an introductory text, uses algebra with optional sections involving calculus)
- Hoiland, Paul (2004). *Preferred Frames of Reference & Relativity*
- Horbatsch, Marko, "Classical Mechanics Course Notes".
- Shapiro, Joel A. (2003). *Classical Mechanics*
- Tong, David. *Classical Dynamics* (Cambridge lecture notes on Lagrangian and Hamiltonian formalism)
- Kinematic Models for Design Digital Library (KMODDL) Movies and photos of hundreds of working mechanical-systems models at Cornell University. Also includes an e-book library of classic texts on mechanical design and engineering.
- MIT OpenCourseWare 8.01: Classical Mechanics Free videos of actual course lectures with links to lecture notes, assignments and exams.
- Alejandro A. Torassa On Classical Mechanics
Chapter 10

Entropy (information theory)

In information theory, entropy is the average amount of information contained in each message received. Here, message stands for an event, sample or character drawn from a distribution or data stream. Entropy thus characterizes our uncertainty about our source of information. (Entropy is best understood as a measure of uncertainty rather than certainty as entropy is larger for more random sources.) The source is also characterized by the probability distribution of the samples drawn from it. The idea here is that the less likely an event is, the more information it provides when it occurs. For some other reasons (explained below) it makes sense to define information as the negative of the logarithm of the probability distribution. The probability distribution of the events, coupled with the information amount of every event, forms a random variable whose average (a.k.a. entropy, generated by this distribution. Because entropy is average information, it is also measured in shannons, nats, or hartleys, depending on the base of the logarithm used to define it.

The logarithm of the probability distribution is useful as a measure of information because it is additive. For instance, flipping a coin provides 1 shannon of information whereas m tosses gather m bits. Generally, you need \( \log_2(n) \) bits to represent a variable that can take one of \( n \) values. Since 1 of \( n \) outcomes is possible when you apply a scale graduated with \( n \) marks, you receive \( \log_2(n) \) bits of information with every such measurement. The \( \log_2(n) \) rule holds only until all outcomes are equally probable. If one of the events occurs more often than others, observation of that event is less informative. Conversely, observing rarer events compensate by providing more information when observed. Since observation of less probable events occurs more rarely, the net effect is that the entropy (thought of as the average information) received from non-uniformly distributed data is less than \( \log_2(n) \).

Entropy is zero when only one certain outcome is expected. Shannon entropy quantifies all these considerations exactly when a probability distribution of the source is provided. It is important to note that the meaning of the events observed (a.k.a. the meaning of messages) do not matter in the definition of entropy. Entropy only takes into account the probability of observing a specific event, so the information it encapsulates is information about the underlying probability distribution, not the meaning of the events themselves.

Generally, “entropy” stands for “disorder” or uncertainty. The entropy we talk about here was introduced by Claude E. Shannon in his 1948 paper ”A Mathematical Theory of Communication”.[1] We also call it Shannon entropy to distinguish from other occurrences of the term, which appears in various parts of physics in different forms. Shannon entropy provides an absolute limit on the best possible average length of lossless encoding or compression of any communication, assuming that\(^2\) the communication may be represented as a sequence of independent and identically distributed random variables.

10.1 Introduction

Entropy is a measure of unpredictability of information content. To get an informal, intuitive understanding of the connection between these three English terms, consider the example of a poll on some political issue. Usually, such polls happen because the outcome of the poll isn’t already known. In other words, the outcome of the poll is relatively unpredictable, and actually performing the poll and learning the results gives some new information; these are just different ways of saying that the entropy of the poll results is large. Now, consider the case that the same poll is performed a second time shortly after the first poll. Since the result of the first poll is already known, the outcome of the second poll can be predicted.
well and the results should not contain much new information; in this case the entropy of the second poll result relative to the first is small.

Now consider the example of a coin toss. When the coin is fair, that is, when the probability of heads is the same as the probability of tails, then the entropy of the coin toss is as high as it could be. This is because there is no way to predict the outcome of the coin toss ahead of time—the best we can do is predict that the coin will come up heads, and our prediction will be correct with probability 1/2. Such a coin toss has one bit of entropy since there are two possible outcomes that occur with equal probability, and learning the actual outcome contains one bit of information. Contrarily, a coin toss with a coin that has two heads and no tails has zero entropy since the coin will always come up heads, and the outcome can be predicted perfectly.

English text has fairly low entropy. In other words, it is fairly predictable. Even if we don’t know exactly what is going to come next, we can be fairly certain that, for example, there will be many more e’s than z’s, that the combination ‘qu’ will be much more common than any other combination with a ‘q’ in it, and that the combination ‘th’ will be more common than ‘th’, ‘q’, or ‘qu’. After the first few letters one can often guess the rest of the word. Uncompressed, English text has between 0.6 and 1.3 bits of entropy for each character of message.\[1\][4]

If a compression scheme is lossless—that is, you can always recover the entire original message by decompressing—then a compressed message has the same quantity of information as the original, but communicated in fewer characters. That is, it has more information, or a higher entropy, per character. This means a compressed message has less redundancy. Roughly speaking, Shannon’s source coding theorem says that a lossless compression scheme cannot compress messages, on average, to have more than one bit of information per bit of message, but that any value less than one bit of information per bit of message can be attained by employing a suitable coding scheme. The entropy of a message per bit multiplied by the length of that message is a measure of how much total information the message contains.

Shannon’s theorem also implies that no lossless compression scheme can shorten all messages. If some messages come out shorter, at least one must come out longer due to the pigeonhole principle. In practical use, this is generally not a problem, because we are usually only interested in compressing certain types of messages, for example English documents as opposed to gibberish text, or digital photographs rather than noise, and it is unimportant if a compression algorithm makes some unlikely or uninteresting sequences larger. However, the problem can still arise even in everyday use when applying a compression algorithm to already compressed data: for example, making a ZIP file of music that is already in the FLAC audio format is unlikely to achieve much extra saving in space.

10.2 Definition

Named after Boltzmann’s H-theorem, Shannon defined the entropy \( H \) (Greek letter Eta) of a discrete random variable \( X \) with possible values \( \{x_1, \ldots, x_n\} \) and probability mass function \( P(X) \) as:

\[
H(X) = E[I(X)] = E[-\ln(P(X))].
\]

Here \( E \) is the expected value operator, and \( I \) is the information content of \( X \).\[5\][6] \( I(X) \) is itself a random variable.

When taken from a finite sample, the entropy can explicitly be written as

\[
H(X) = \sum_{i} P(x_i) I(x_i) = -\sum_{i} P(x_i) \log_b P(x_i)
\]

where \( b \) is the base of the logarithm used. Common values of \( b \) are 2, Euler’s number \( e \), and 10, and the unit of entropy is shannon for \( b = 2 \), nat for \( b = e \), and hartley for \( b = 10 \).\[7]

In the case of \( p(x_i) = 0 \) for some \( i \), the value of the corresponding summand \( 0 \log_b(0) \) is taken to be 0, which is consistent with the well-known limit:

\[
\lim_{p \to 0^+} p \log(p) = 0
\]

One may also define the conditional entropy of two events \( X \) and \( Y \) taking values \( x_i \) and \( y_j \) respectively, as

\[
H(X|Y) = \sum_{i,j} p(x_i, y_j) \log \frac{p(y_j)}{p(x_i, y_j)}
\]

where \( p(x_i, y_j) \) is the probability that \( X = x_i \) and \( Y = y_j \). This quantity should be understood as the amount of randomness in the random variable \( X \) given that you know the value of \( Y \).

10.3 Example

Main article: Binary entropy function
Main article: Bernoulli process

Consider tossing a coin with known, not necessarily fair, probabilities of coming up heads or tails; this is known as the Bernoulli process. The entropy of the unknown result of the next toss of the coin is maximized if the coin is fair (that is, if heads and tails both have equal probability 1/2). This is the situation of maximum uncertainty as it is most difficult to predict
10.5. ASPECTS

1. **Entropy** $H(X)$ (i.e. the expected surprisal) of a coin flip, measured in shannons, graphed versus the fairness of the coin $P(X=1)$, where $X=1$ represents a result of heads.

Note that the maximum of the graph depends on the distribution. Here, the entropy is at most 1 shannon, and to communicate the outcome of a fair coin flip (2 possible values) will require an average of at most 1 bit. The result of a fair die (6 possible values) would require an average $\log_2 6$ bits.

However, if we know the coin is not fair, but comes up heads with probabilities $p$ and $q$, where $p \neq q$, there is less uncertainty. Every time it is tossed, one side is more likely to come up than the other. The reduced uncertainty is quantified in a lower entropy: on average each toss of the coin delivers less than one full bit of information.

The extreme case is that of a double-headed coin that never comes up tails, or a double-tailed coin that never results in a head. Then there is no uncertainty. The entropy is zero: each toss of the coin delivers no new information as the outcome of each coin toss is always certain. In this respect, entropy can be normalized by dividing it by information length. This ratio is called metric entropy and is a measure of the randomness of the information.

10.4 Rationale

To understand the meaning of $\sum p_i \log \frac{1}{p_i}$, at first, try to define an information function, $I$, in terms of an event $i$ with probability $p_i$. How much information is acquired due to the observation of event $i$? Shannon’s solution follows from the fundamental properties of information. [8]

1. $I(p) \geq 0$ – information is a non-negative quantity
2. $I(1) = 0$ – events that always occur do not communicate information
3. $I(p_1, p_2) = I(p_1) + I(p_2)$ – information due to independent events is additive

The latter is a crucial property. It states that joint probability communicates as much information as two individual events separately. Particularly, if the first event can yield one of $n$ equiprobable outcomes and another has one of $m$ equiprobable outcomes then there are $mn$ possible outcomes of the joint event. This means that if $\log_2 (n)$ bits are needed to encode the first value and $\log_2 (m)$ to encode the second, one needs $\log_2 (mn) = \log_2 (m) + \log_2 (n)$ to encode both. Shannon discovered that the proper choice of function to quantify information, preserving this additivity, is logarithmic, i.e.,

$I(p) = \log(1/p)$

The base of logarithm does not matter; any can be used. The different units of information (bits for $\log_2$, trits for $\log_3$, nats for $\ln$ and so on) are just constant multiples of each other. For instance, in case of a fair coin toss, heads provides $\log_2 (2) = 1$ bit of information. Because of additivity, $n$ tosses provide $n$ bits of information.

Now, suppose we have a distribution where event $i$ can happen with probability $p_i$. Suppose we have sampled it $N$ times and outcome $i$ was, accordingly, seen $n_i = N p_i$ times. The total amount of information we have received is

$$\sum_i n_i I(p_i) = \sum_i N p_i \log(1/p_i)$$

The average amount of information that we receive with every event is therefore

$$\sum_i p_i \log \frac{1}{p_i}.$$
\[ S = -k_B \sum p_i \ln p_i \]

where \( k_B \) is the Boltzmann constant, and \( p_i \) is the probability of a microstate. The Gibbs entropy was defined by J. Willard Gibbs in 1878 after earlier work by Boltzmann (1872).\(^9\)

The Gibbs entropy translates over almost unchanged into the world of quantum physics to give the von Neumann entropy, introduced by John von Neumann in 1927.

\[ S = -k_B \text{Tr}(\rho \ln \rho) \]

where \( \rho \) is the density matrix of the quantum mechanical system and \( \text{Tr} \) is the trace.

At an everyday practical level the links between information entropy and thermodynamic entropy are not evident. Physicists and chemists are apt to be more interested in changes in entropy as a system spontaneously evolves away from its initial conditions, in accordance with the second law of thermodynamics, rather than an unchanging probability distribution. And, as the minuteness of Boltzmann’s constant \( k_B \) indicates, the changes in \( S/k_B \) for even tiny amounts of substances in chemical and physical processes represent amounts of entropy that are extremely large compared to anything in data compression or signal processing. Furthermore, in classical thermodynamics the entropy is defined in terms of macroscopic measurements and makes no reference to any probability distribution, which is central to the definition of information entropy.

At a multidisciplinary level, however, connections can be made between thermodynamic and informational entropy, although it took many years in the development of the theories of statistical mechanics and information theory to make the relationship fully apparent. In fact, in the view of Jaynes (1957), thermodynamic entropy, as explained by statistical mechanics, should be seen as an application of Shannon’s information theory: the thermodynamic entropy is interpreted as being proportional to the amount of further Shannon information needed to define the detailed microscopic state of the system, that remains uncommunicated by a description solely in terms of the macroscopic variables of classical thermodynamics, with the constant of proportionality being just the Boltzmann constant. For example, adding heat to a system increases its thermodynamic entropy because it increases the number of possible microscopic states of the system that are consistent with the measurable values of its macroscopic variables, thus making any complete state description longer. (See article: maximum entropy thermodynamics). Maxwell’s demon can (hypothetically) reduce the thermodynamic entropy of a system by using information about the states of individual molecules; but, as Landauer (from 1961) and co-workers have shown, to function the demon himself must increase thermodynamic entropy in the process, by at least the amount of Shannon information he proposes to first acquire and store; and so the total thermodynamic entropy does not decrease (which resolves the paradox). Landauer’s principle has implications on the amount of heat a computer must dissipate to process a given amount of information, though modern computers are nowhere near the efficiency limit.

### 10.5.2 Entropy as information content

Main article: Shannon’s source coding theorem

Entropy is defined in the context of a probabilistic model. Independent fair coin flips have an entropy of 1 bit per flip. A source that always generates a long string of B’s has an entropy of 0, since the next character will always be a ‘B’.

The entropy rate of a data source means the average number of bits per symbol needed to encode it. Shannon’s experiments with human predictors show an information rate between 0.6 and 1.3 bits per character in English,\(^{10}\) the PPM compression algorithm can achieve a compression ratio of 1.5 bits per character in English text.

From the preceding example, note the following points:

1. The amount of entropy is not always an integer number of bits.
2. Many data bits may not convey information. For example, data structures often store information redundantly, or have identical sections regardless of the information in the data structure.

Shannon’s definition of entropy, when applied to an information source, can determine the minimum channel capacity required to reliably transmit the source as encoded binary digits (see caveat below in italics). The formula can be derived by calculating the mathematical expectation of the amount of information contained in a digit from the information source. See also Shannon-Hartley theorem.

Shannon’s entropy measures the information contained in a message as opposed to the portion of the message that is determined (or predictable). Examples of the latter include redundancy in language structure or statistical properties relating to the occurrence frequencies of letter or word pairs, triplets etc. See Markov chain.

### 10.5.3 Data compression

Main article: Data compression

Entropy effectively bounds the performance of the strongest lossless compression possible, which can be realized in theory by using the typical set or in practice us-
ing Huffman, Lempel-Ziv or arithmetic coding. The performance of existing data compression algorithms is often used as a rough estimate of the entropy of a block of data.\[11\][12] See also Kolmogorov complexity. In practice, compression algorithms deliberately include some judicious redundancy in the form of checksums to protect against errors.

10.5.4 World’s technological capacity to store and communicate entropic information

A 2011 study in Science estimates the world’s technological capacity to store and communicate optimally compressed information normalized on the most effective compression algorithms available in the year 2007, therefore estimating the entropy of the technologically available sources.\[13\]

The authors estimate humankind technological capacity to store information (fully entropically compressed) in 1986 and again in 2007. They break the information into three categories - To store information on a medium, to receive information through a one-way broadcast networks, to exchange information through two-way telecommunication networks.\[13\]

10.5.5 Limitations of entropy as information content

There are a number of entropy-related concepts that mathematically quantify information content in some way:

- the self-information of an individual message or symbol taken from a given probability distribution,
- the entropy of a given probability distribution of messages or symbols, and
- the entropy rate of a stochastic process.

(The “rate of self-information” can also be defined for a particular sequence of messages or symbols generated by a given stochastic process: this will always be equal to the entropy rate in the case of a stationary process.) Other quantities of information are also used to compare or relate different sources of information.

It is important not to confuse the above concepts. Often it is only clear from context which one is meant. For example, when someone says that the “entropy” of the English language is about 1 bit per character, they are actually modeling the English language as a stochastic process and talking about its entropy rate.

Although entropy is often used as a characterization of the information content of a data source, this information content is not absolute: it depends crucially on the probabilistic model. A source that always generates the same symbol has an entropy rate of 0, but the definition of what a symbol is depends on the alphabet. Consider a source that produces the string AABABABAB... in which A is always followed by B and vice versa. If the probabilistic model considers individual letters as independent, the entropy rate of the sequence is 1 bit per character. But if the sequence is considered as “AB AB AB AB AB...” with symbols as two-character blocks, then the entropy rate is 0 bits per character.

However, if we use very large blocks, then the estimate of per-character entropy rate may become artificially low. This is because in reality, the probability distribution of the sequence is not knowable exactly; it is only an estimate. For example, suppose one considers the text of every book ever published as a sequence, with each symbol being the text of a complete book. If there are \(N\) published books, and each book is only published once, the estimate of the probability of each book is \(1/N\), and the entropy (in bits) is \(-\log_2(1/N) = \log_2(N)\). As a practical code, this corresponds to assigning each book a unique identifier and using it in place of the text of the book whenever one wants to refer to the book. This is enormously useful for talking about books, but it is not so useful for characterizing the information content of an individual book, or of language in general: it is not possible to reconstruct the book from its identifier without knowing the probability distribution, that is, the complete text of all the books. The key idea is that the complexity of the probabilistic model must be considered. Kolmogorov complexity is a theoretical generalization of this idea that allows the consideration of the information content of a sequence independent of any particular probability model; it considers the shortest program for a universal computer that outputs the sequence. A code that achieves the entropy rate of a sequence for a given model, plus the codebook (i.e. the probabilistic model), is one such program, but it may not be the shortest.

For example, the Fibonacci sequence is 1, 1, 2, 3, 5, 8, 13, \ldots. Treating the sequence as a message and each number as a symbol, there are almost as many symbols as there are characters in the message, giving an entropy of approximately \(\log_2(n)\). So the first 128 symbols of the Fibonacci sequence has an entropy of approximately 7 bits/symbol. However, the sequence can be expressed using a formula \[F(n) = F(n-1) + F(n-2)\] for \(n=\{3,4,5,\ldots\}\), \(F(1)=1, F(2)=1\) and this formula has a much lower entropy and applies to any length of the Fibonacci sequence.

10.5.6 Limitations of entropy as a measure of unpredictability

In cryptanalysis, entropy is often roughly used as a measure of the unpredictability of a cryptographic key. For example, a 128-bit key that is randomly generated has
128 bits of entropy. It takes (on average) $2^{128-1}$ guesses to break by brute force. If the key’s first digit is 0, and the others random, then the entropy is 127 bits, and it takes (on average) $2^{127-1}$ guesses.

However, entropy fails to capture the number of guesses required if the possible keys are not of equal probability. If the key is half the time “password” and half the time a true random 128-bit key, then the entropy is approximately 65 bits. Yet half the time the key may be guessed on the first try, if your first guess is “password”, and on average, it takes around $2^{126}$ guesses (not $2^{65-1}$) to break this password.

Similarly, consider a 1000000-digit binary one-time pad. If the pad has 1000000 bits of entropy, it is perfect. If the pad has 999999 bits of entropy, evenly distributed (each individual bit of the pad having 0.999999 bits of entropy) it may still be considered very good. But if the pad has 999999 bits of entropy, where the first digit is fixed and the remaining 999999 digits are perfectly random, then the first digit of the ciphertext will not be encrypted at all.

### 10.5.7 Data as a Markov process

A common way to define entropy for text is based on the Markov model of text. For an order-0 source (each character is selected independent of the last characters), the binary entropy is:

$$H(S) = - \sum_i p_i \log_2 p_i,$$

where $p_i$ is the probability of $i$. For a first-order Markov source (one in which the probability of selecting a character is dependent only on the immediately preceding character), the entropy rate is:

$$H(S) = - \sum_i p_i \sum_j p_i(j) \log_2 p_i(j),$$

where $i$ is a state (certain preceding characters) and $p_i(j)$ is the probability of $j$ given $i$ as the previous character.

For a second order Markov source, the entropy rate is

$$H(S) = - \sum_i p_i \sum_j p_i(j) \sum_k p_i,j(k) \log_2 p_i,j(k).$$

### 10.5.8 b-ary entropy

In general the b-ary entropy of a source $S = (S,P)$ with source alphabet $S = \{a_1, \ldots, a_n\}$ and discrete probability distribution $P = \{p_1, \ldots, p_n\}$ where $p_i$ is the probability of $ai$ (say $p_i = p(ai)$) is defined by:

$$H_b(S) = - \sum_{i=1}^n p_i \log_b p_i.$$
10.8. FURTHER PROPERTIES

10.7.2 Symmetry

The measure should be unchanged if the outcomes $x_i$ are re-ordered.

$$H_n(p_1, p_2, \ldots) = H_n(p_2, p_1, \ldots)$$

10.7.3 Maximum

The measure should be maximal if all the outcomes are equally likely (uncertainty is highest when all possible events are equiprobable).

$$H_n(p_1, \ldots, p_n) \leq H_n\left(\frac{1}{n}, \ldots, \frac{1}{n}\right) = \log_b(n).$$

For equiprobable events the entropy should increase with the number of outcomes.

$$H_n\left(\frac{1}{n}, \ldots, \frac{1}{n}\right) = \log_b(n) < \log_b(n+1) = H_{n+1}\left(\frac{1}{n+1}, \ldots, \frac{1}{n+1}\right).$$

10.7.4 Additivity

The amount of entropy should be independent of how the process is regarded as being divided into parts.

This last functional relationship characterizes the entropy of a system with sub-systems. It demands that the entropy of a system can be calculated from the entropies of its sub-systems if the interactions between the sub-systems are known.

Given an ensemble of $n$ uniformly distributed elements that are divided into $k$ boxes (sub-systems) with $b_1, \ldots, b_k$ elements each, the entropy of the whole ensemble should be equal to the sum of the entropy of the system of boxes and the individual entropies of the boxes, each weighted with the probability of being in that particular box.

For positive integers $b_i$ where $b_1 + \ldots + b_k = n$,

$$H_n\left(\frac{1}{n}, \ldots, \frac{1}{n}\right) = H_k\left(\frac{b_1}{n}, \ldots, \frac{b_k}{n}\right) + \sum_{i=1}^{k} b_i H_{b_i}\left(\frac{1}{b_i}, \ldots, \frac{1}{b_i}\right).$$

Choosing $k = n$, $b_1 = \ldots = b_n = 1$ this implies that the entropy of a certain outcome is zero: $H_1(1) = 0$. This implies that the efficiency of a source alphabet with $n$ symbols can be defined simply as being equal to its $n$-ary entropy. See also Redundancy (information theory).

10.8 Further properties

The Shannon entropy satisfies the following properties, for some of which it is useful to interpret entropy as the amount of information learned (or uncertainty eliminated) by revealing the value of a random variable $X$:

- Adding or removing an event with probability zero does not contribute to the entropy:

$$H_{n+1}(p_1, \ldots, p_n, 0) = H_n(p_1, \ldots, p_n)$$

- It can be confirmed using the Jensen inequality that

$$H(X) = \mathbb{E} \left[ \log_b\left(\frac{1}{p(X)}\right) \right] \leq \log_b \left( \mathbb{E} \left[ \frac{1}{p(X)} \right] \right) = \log_b(n)$$

This maximal entropy of $\log_b(n)$ is effectively attained by a source alphabet having a uniform probability distribution: uncertainty is maximal when all possible events are equiprobable.

The entropy or the amount of information revealed by evaluating $(X, Y)$ (that is, evaluating $X$ and $Y$ simultaneously) is equal to the information revealed by conducting two consecutive experiments: first evaluating the value of $Y$, then revealing the value of $X$ given that you know the value of $Y$. This may be written as

$$H[(X, Y)] = H(X|Y) + H(Y) = H(Y|X) + H(X).$$

- If $Y = f(X)$ where $f$ is deterministic, then $H(f(X)|X) = 0$. Applying the previous formula to $H(X, f(X))$ yields

$$H(X) + H(f(X)|X) = H(f(X)) + H(X|f(X)),$$

so $H(f(X)) \leq H(X)$, thus the entropy of a variable can only decrease when the latter is passed through a deterministic function.

- If $X$ and $Y$ are two independent experiments, then knowing the value of $Y$ doesn’t influence our knowledge of the value of $X$ (since the two don’t influence each other by independence):

$$H(X|Y) = H(X).$$
The entropy of two simultaneous events is no more than the sum of the entropies of each individual event, and are equal if the two events are independent. More specifically, if \( X \) and \( Y \) are two random variables on the same probability space, and \((X, Y)\) denotes their Cartesian product, then

\[
H[(X, Y)] \leq H(X) + H(Y).
\]

Proving this mathematically follows easily from the previous two properties of entropy.

### 10.9 Extending discrete entropy to the continuous case

#### 10.9.1 Differential entropy

Main article: Differential entropy

The Shannon entropy is restricted to random variables taking discrete values. The corresponding formula for a continuous random variable with probability density function \( f(x) \) with finite or infinite support \( \mathbb{X} \) on the real line is defined by analogy, using the above form of the entropy as an expectation:

\[
h[f] = E[-\ln(f(x))] = -\int_{\mathbb{X}} f(x) \ln(f(x)) \, dx.
\]

This formula is usually referred to as the continuous entropy, or differential entropy. A precursor of the continuous entropy \( h[f] \) is the expression for the functional \( H \) in the H-theorem of Boltzmann.

Although the analogy between both functions is suggestive, the following question must be set: is the differential entropy a valid extension of the Shannon discrete entropy? Differential entropy lacks a number of properties that the Shannon discrete entropy has – it can even be negative – and thus corrections have been suggested, notably limiting density of discrete points.

To answer this question, we must establish a connection between the two functions:

We wish to obtain a generally finite measure as the bin size goes to zero. In the discrete case, the bin size is the (implicit) width of each of the \( n \) (finite or infinite) bins whose probabilities are denoted by \( p_m \). As we generalize to the continuous domain, we must make this width explicit.

To do this, start with a continuous function \( f \) discretized into bins of size \( \Delta \). By the mean-value theorem there exists a value \( x_i \) in each bin such that

\[
f(x_i)\Delta = \int_{i\Delta}^{(i+1)\Delta} f(x) \, dx
\]

and thus the integral of the function \( f \) can be approximated (in the Riemannian sense) by

\[
\int_{-\infty}^{\infty} f(x) \, dx = \lim_{\Delta \to 0} \sum_{i=-\infty}^{\infty} f(x_i)\Delta
\]

where this limit and “bin size goes to zero” are equivalent. We will denote

\[
H^\Delta := -\sum_{i=-\infty}^{\infty} f(x_i)\Delta \log(f(x_i)\Delta)
\]

and expanding the logarithm, we have

\[
H^\Delta = -\sum_{i=-\infty}^{\infty} f(x_i)\Delta \log(f(x_i)) - \sum_{i=-\infty}^{\infty} f(x_i)\Delta \log(\Delta).
\]

As \( \Delta \to 0 \), we have

\[
\sum_{i=-\infty}^{\infty} f(x_i)\Delta \to \int_{-\infty}^{\infty} f(x) \, dx = 1
\]

\[
\sum_{i=-\infty}^{\infty} f(x_i)\Delta \log(f(x_i)) \to \int_{-\infty}^{\infty} f(x) \log f(x) \, dx.
\]

But note that \( \log(\Delta) \to -\infty \) as \( \Delta \to 0 \), therefore we need a special definition of the differential or continuous entropy:

\[
h[f] = \lim_{\Delta \to 0} (H^\Delta + \log \Delta) = -\int_{-\infty}^{\infty} f(x) \log f(x) \, dx,
\]

which is, as said before, referred to as the differential entropy. This means that the differential entropy is not a limit of the Shannon entropy for \( n \to \infty \). Rather, it differs from the limit of the Shannon entropy by an infinite offset.

It turns out as a result that, unlike the Shannon entropy, the differential entropy is not in general a good measure of uncertainty or information. For example, the differential entropy can be negative; also it is not invariant under continuous co-ordinate transformations.

#### 10.9.2 Relative entropy

Main article: Generalized relative entropy

Another useful measure of entropy that works equally well in the discrete and the continuous case is the relative
entropy of a distribution. It is defined as the Kullback–Leibler divergence from the distribution to a reference measure \( m \) as follows. Assume that a probability distribution \( p \) is absolutely continuous with respect to a measure \( m \), i.e. is of the form \( p(dx) = f(x)m(dx) \) for some non-negative \( m \)-integrable function \( f \) with \( m \)-integral 1, then the relative entropy can be defined as

\[
D_{KL}(p|m) = \int \log(f(x))p(dx) = \int f(x)\log(f(x))m(dx).
\]

In this form the relative entropy generalises (up to change in sign) both the discrete entropy, where the measure \( m \) is the counting measure, and the differential entropy, where the measure \( m \) is the Lebesgue measure. If the measure \( m \) is itself a probability distribution, the relative entropy is non-negative, and zero if \( p \) is itself a probability distribution, the relative entropy \( H \) and \( m \) are subsets of \( \{1, \ldots, d\} \), then equality holds if and only if \( p = m \).

A simple example of this is an alternate proof of the Loomis-Whitney inequality: for any subset \( A \subseteq \mathbb{Z}^d \), we have

\[
|A|^{d-1} \leq \prod_{i=1}^{d} |P_i(A)|
\]

where \( P_i \) is the orthogonal projection in the \( i \)th coordinate:

\[
P_i(A) = \{(x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_d) : (x_1, \ldots, x_d) \in A \}.
\]

The proof follows as a simple corollary of Shearer’s inequality: if \( X_1, \ldots, X_d \) are random variables and \( S_1, \ldots, S_n \) are subsets of \( \{1, \ldots, d\} \) such that every integer between \( 1 \) and \( d \) lies in exactly \( r \) of these subsets, then

\[
H[(X_1, \ldots, X_d)] \leq \frac{1}{r} \sum_{i=1}^{n} H[(X_j)_{j \in S_i}]
\]

where \( (X_j)_{j \in S_i} \) is the Cartesian product of random variables \( X_j \) with indexes \( j \) in \( S_i \) (so the dimension of this vector is equal to the size of \( S_i \)).

We sketch how Loomis-Whitney follows from this: Indeed, let \( X \) be a uniformly distributed random variable with values in \( A \) and so that each point in \( A \) occurs with equal probability. Then (by the further properties of entropy mentioned above) \( H(X) = \log|A| \), where \(|A|\) denotes the cardinality of \( A \). Let \( S_i = \{1, 2, \ldots, i-1, i+1, \ldots, d\} \). The range of \( (X_j)_{j \in S_i} \) is contained in \( P(A) \) and hence \( H[(X_j)_{j \in S_i}] \leq \log |P(A)| \). Now use this to bound the right side of Shearer’s inequality and exponentiate the opposite sides of the resulting inequality you obtain.

### 10.10 Use in combinatorics

Entropy has become a useful quantity in combinatorics.

#### 10.10.1 Loomis-Whitney inequality

A simple example of this is an alternate proof of the Loomis-Whitney inequality: for every subset \( A \subseteq \mathbb{Z}^d \), we have

\[
\sum_{i=0}^{n} \binom{n}{i} q^i (1-q)^{n-i} = (q + (1-q))^n = 1.
\]

Rearranging gives the upper bound. For the lower bound one first shows, using some algebra, that it is the largest term in the summation. But then,

\[
\binom{n}{k} q^k (1-q)^{n-k} \geq \frac{1}{n+1}
\]

since there are \( n+1 \) terms in the summation. Rearranging gives the lower bound.

A nice interpretation of this is that the number of binary strings of length \( n \) with exactly \( k \) many 1’s is approximately \( 2^{nH(k/n)} \).

### 10.11 See also

- Conditional entropy
- Cross entropy – is a measure of the average number of bits needed to identify an event from a set of possibilities between two probability distributions
- Entropy (arrow of time)
- Entropy encoding – a coding scheme that assigns codes to symbols so as to match code lengths with the probabilities of the symbols.
• Entropy estimation
• Entropy power inequality
• Entropy rate
• Fisher information
• Hamming distance
• History of entropy
• History of information theory
• Information geometry
• Joint entropy – is the measure how much entropy is contained in a joint system of two random variables.
• Kolmogorov-Sinai entropy in dynamical systems
• Levenshtein distance
• Mutual information
• Negentropy
• Perplexity
• Qualitative variation – other measures of statistical dispersion for nominal distributions
• Quantum relative entropy – a measure of distinguishability between two quantum states.
• Rényi entropy – a generalisation of Shannon entropy; it is one of a family of functionals for quantifying the diversity, uncertainty or randomness of a system.
• Shannon index
• Theil index
• Typoglycemia

10.12 References


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10.13 Further reading

10.13.1 Textbooks on information theory


### 10.14 External links

• *Entropy* an interdisciplinary journal on all aspect of the entropy concept. Open access.

• Information is not entropy, information is not uncertainty! – a discussion of the use of the terms “information” and “entropy”.

• I’m Confused: How Could Information Equal Entropy? – a similar discussion on the bionet.info-theory FAQ.

• Description of information entropy from “Tools for Thought” by Howard Rheingold

• A java applet representing Shannon’s Experiment to Calculate the Entropy of English

• Slides on information gain and entropy

• *An Intuitive Guide to the Concept of Entropy Arising in Various Sectors of Science* – a wikibook on the interpretation of the concept of entropy.

• Calculator for Shannon entropy estimation and interpretation

• A Light Discussion and Derivation of Entropy

• Network Event Detection With Entropy Measures, Dr. Raimund Eimann, University of Auckland, PDF; 5993 kB – a PhD thesis demonstrating how entropy measures may be used in network anomaly detection.
Chapter 11

Topological entropy

This article is about entropy in geometry and topology. For other uses, see Entropy (disambiguation).

In mathematics, the topological entropy of a topological dynamical system is a nonnegative real number that is a measure of the complexity of the system. Topological entropy was first introduced in 1965 by Adler, Konheim and McAndrew. Their definition was modelled after the definition of the Kolmogorov–Sinai, or metric entropy. Later, Dinaburg and Rufus Bowen gave a different, weaker definition reminiscent of the Hausdorff dimension. The second definition clarified the meaning of the topological entropy: for a system given by an iterated function, the topological entropy represents the exponential growth rate of the number of distinguishable orbits of the iterates. An important variational principle relates the notions of topological and measure-theoretic entropy.

11.1 Definition

A topological dynamical system consists of a Hausdorff topological space $X$ (usually assumed to be compact) and a continuous self-map $f$. Its topological entropy is a non-negative real number that can be defined in various ways, which are known to be equivalent.

11.1.1 Definition of Adler, Konheim, and McAndrew

Let $X$ be a compact Hausdorff topological space. For any finite open cover $C$ of $X$, let $H(C)$ be the logarithm (usually to base 2) of the smallest number of elements of $C$ that cover $X$. For two covers $C$ and $D$, let

$$H(C, f) = \lim_{n \to \infty} \frac{1}{n} H(C \lor f^{-1}C \lor \ldots \lor f^{-n+1}C).$$

Then the topological entropy of $f$, denoted $h(f)$, is defined to be the supremum of $H(C, f)$ over all possible finite covers $C$ of $X$.

Interpretation

The parts of $C$ may be viewed as symbols that (partially) describe the position of a point $x$ in $X$: all points $x \in Ci$ are assigned the symbol $Ci$. Imagine that the position of $x$ is (imperfectly) measured by a certain device and that each part of $C$ corresponds to one possible outcome of the measurement. The integer $H(C \lor f^{-1}C \lor \ldots \lor f^{-n+1}C)$ then represents the minimal number of “words” of length $n$ needed to encode the points of $X$ according to the behavior of their first $n - 1$ iterates under $f$, or, put differently, the total number of “scenarios” of the behavior of these iterates, as “seen” by the partition $C$. Thus the topological entropy is the average (per iteration) amount of information needed to describe long iterations of the map $f$.

11.1.2 Definition of Bowen and Dinaburg

This definition uses a metric on $X$ (actually, uniform structure would suffice). This is a weaker definition than that of Adler, Konheim, and McAndrew, as it requires additional, unnecessary structure on the topological space. However, in practice, the Bowen-Dinaburg topological entropy is usually much easier to calculate.

Let $(X, d)$ be a compact metric space and $f : X \to X$ be a continuous map. For each natural number $n$, a new metric $d_n$ is defined on $X$ by the formula

$$d_n(x, y) = \max \{ d(f^i(x), f^i(y)) : 0 \leq i < n \}.$$ 

Given any $\varepsilon > 0$ and $n \geq 1$, two points of $X$ are $\varepsilon$-close with respect to this metric if their first $n$ iterates are $\varepsilon$-close. This metric allows one to distinguish in a neighborhood
of an orbit the points that move away from each other during the iteration from the points that travel together. A subset $E$ of $X$ is said to be $(n, \varepsilon)$-separated if each pair of distinct points of $E$ is at least $\varepsilon$ apart in the metric $d$. Denote by $N(n, \varepsilon)$ the maximum cardinality of an $(n, \varepsilon)$-separated set. The **topological entropy** of the map $f$ is defined by

$$h(f) = \lim_{\varepsilon \to 0} \left( \lim_{n \to \infty} \frac{1}{n} \log N(n, \varepsilon) \right).$$

**Interpretation**

Since $X$ is compact, $N(n, \varepsilon)$ is finite and represents the number of distinguishable orbit segments of length $n$, assuming that we cannot distinguish points within $\varepsilon$ of one another. A straightforward argument shows that the limit defining $h(f)$ always exists in the extended real line (but could be infinite). This limit may be interpreted as the measure of the average exponential growth of the number of distinguishable orbit segments. In this sense, it measures complexity of the topological dynamical system $(X, f)$. Rufus Bowen extended this definition of topological entropy in a way which permits $X$ to be noncompact.

### 11.2 Properties

- Let $f$ be an expansive homeomorphism of a compact metric space $X$ and let $C$ be a topological generator. Then the topological entropy of $f$ relative to $C$ is equal to the topological entropy of $f$, i.e.

$$h(f) = H(f, C)$$

- Let $f : X \to X$ be a continuous transformation of a compact metric space $X$, let $h_\mu(f)$ be the measure-theoretic entropy of $f$ with respect to $\mu$ and $M(X, f)$ is the set of all $f$-invariant Borel probability measures. Then

$$h(f) = \sup_{\mu \in M(X, f)} h_\mu(f)$$

- In general the maximum of the functions $h_\mu$ over the set $M(X,f)$ is not attained, but if additionally the entropy map

$$\mu \mapsto h_\mu(f) : M(X, f) \to \mathbb{R}$$

is upper semi-continuous, the measure of maximal entropy exists.

- If $f$ has a unique measure of maximal entropy $\mu$, then $f$ is ergodic with respect to $\mu$.

### 11.3 Examples

- Let $\sigma : \Sigma_k \to \Sigma$ by $x_n \mapsto x_{n-1}$ denote the full two-sided $k$-shift on symbols $\{1, \ldots, k\}$. Let $C = \{[1], \ldots, [k]\}$ denote the partition of $\Sigma_k$ into cylinders of length 1. Then $\bigvee_{j=0}^n \sigma^{-1}(C)$ is a partition of $\Sigma_k$ for all $n \in \mathbb{N}$ and the number of sets is $k^n$ respectively. The partitions are open covers and $C$ is a topological generator. Hence

$$h(\sigma) = h(\sigma, C) = \lim_{n \to \infty} \frac{1}{n} \log k^n = \log k.$$  The measure-theoretic entropy of the Bernoulli $(\frac{1}{k}, \ldots, \frac{1}{k})$-measure is also $\log k$. Hence it is a measure of maximal entropy. Further on it can be shown that no other measures of maximal entropy exist.

- Let $A$ be an irreducible $k \times k$ matrix with entries in $\{0, 1\}$ and let $\sigma : \Sigma_A \to \Sigma_A$ be the corresponding subshift of finite type. Then $h(\sigma) = \log \lambda$ where $\lambda$ is the largest positive eigenvalue of $A$.

### 11.4 Notes

[1] Since $X$ is compact, $H(C)$ is always finite, even for an infinite cover $C$. The use of arbitrary covers yields the same value of entropy.

### 11.5 See also

- Milnor–Thurston kneading theory
- For the measure of correlations in systems with topological order see Topological entanglement entropy

### 11.6 References

- Roy Adler, Tomasz Downarowicz, Michał Misiurewicz, Topological entropy at Scholarpedia
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Chapter 12

Measure-preserving dynamical system

In mathematics, a measure-preserving dynamical system is an object of study in the abstract formulation of dynamical systems, and ergodic theory in particular.

12.1 Definition

A measure-preserving dynamical system is defined as a probability space and a measure-preserving transformation on it. In more detail, it is a system

\[(X, \mathcal{B}, \mu, T)\]

with the following structure:

- \(X\) is a set,
- \(\mathcal{B}\) is a \(\sigma\)-algebra over \(X\),
- \(\mu : \mathcal{B} \to [0, 1]\) is a probability measure, so that \(\mu(X) = 1\), and \(\mu(\emptyset) = 0\),
- \(T : X \to X\) is a measurable transformation which preserves the measure \(\mu\), i.e., \(\forall A \in \mathcal{B} \mu(T^{-1}(A)) = \mu(A)\).

This definition can be generalized to the case in which \(T\) is not a single transformation that is iterated to give the dynamics of the system, but instead is a monoid (or even a group) of transformations \(T_s : X \to X\) parametrized by \(s \in \mathbb{Z}\) (or \(\mathbb{R}\), or \(\mathbb{N} \cup \{0\}\), or \([0, +\infty)\)), where each transformation \(T_s\) satisfies the same requirements as \(T\) above. In particular, the transformations obey the rules:

- \(T_0 = id_X : X \to X\), the identity function on \(X\);
- \(T_s \circ T_t = T_{t+s}\), whenever all the terms are well-defined;
- \(T_s^{-1} = T_{-s}\), whenever all the terms are well-defined.

Examples include:

- \(\mu\) could be the normalized angle measure \(d\theta/2\pi\) on the unit circle, and \(T\) a rotation. See equidistribution theorem;
- the Bernoulli scheme;
- the interval exchange transformation;
- with the definition of an appropriate measure, a subshift of finite type;
- the base flow of a random dynamical system.

12.3 Homomorphisms

The concept of a homomorphism and an isomorphism may be defined.
Consider two dynamical systems \((X, A, \mu, T)\) and \((Y, B, \nu, S)\). Then a mapping
\[
\varphi : X \to Y
\]
is a **homomorphism of dynamical systems** if it satisfies the following three properties:

1. The map \(\varphi\) is measurable,
2. For each \(B \in B\), one has \(\mu(\varphi^{-1}B) = \nu(B)\),
3. For \(\mu\)-almost all \(x \in X\), one has \(\varphi(Tx) = S(\varphi x)\).

The system \((Y, B, \nu, S)\) is then called a **factor** of \((X, A, \mu, T)\).

The map \(\varphi\) is an **isomorphism of dynamical systems** if, in addition, there exists another mapping
\[
\psi : Y \to X
\]
that is also a homomorphism, which satisfies

1. For \(\mu\)-almost all \(x \in X\), one has \(x = \psi(\varphi x)\).
2. For \(\nu\)-almost all \(y \in Y\), one has \(y = \varphi(\psi y)\).

Hence, one may form a category of dynamical systems and their homomorphisms.

### 12.4 Generic points

A point \(x \in X\) is called a **generic point** if the orbit of the point is distributed uniformly according to the measure.

### 12.5 Symbolic names and generators

Consider a dynamical system \((X, B, T, \mu)\), and let \(Q = \{Q_1, \ldots, Q_k\}\) be a partition of \(X\) into \(k\) measurable pairwise disjoint pieces. Given a point \(x \in X\), clearly \(x\) belongs to only one of the \(Q_i\). Similarly, the iterated point \(T^n x\) can belong to only one of the parts as well. The **symbolic name** of \(x\), with regards to the partition \(Q\), is the sequence of integers \(\{an\}\) such that
\[
T^n x \in Q_{a_n}.
\]

The set of symbolic names with respect to a partition is called the **symbolic dynamics** of the dynamical system. A partition \(Q\) is called a **generator** or **generating partition** if \(\mu\)-almost every point \(x\) has a unique symbolic name.

### 12.6 Operations on partitions

Given a partition \(Q = \{Q_1, \ldots, Q_k\}\) and a dynamical system \((X, B, T, \mu)\), we define \(T\)-pullback of \(Q\) as
\[
T^{-1}Q = \{T^{-1}Q_1, \ldots, T^{-1}Q_k\}.
\]

Further, given two partitions \(Q = \{Q_1, \ldots, Q_k\}\) and \(R = \{R_1, \ldots, R_m\}\), we define their refinement as
\[
Q \lor R = \{Q_i \cap R_j \mid i = 1, \ldots, k, j = 1, \ldots, m, \mu(Q_i \cap R_j) > 0\}.
\]

With these two constructs we may define **refinement of an iterated pullback**
\[
\bigvee_{n=0}^{N} T^{-n}Q = \bigcup_{n=0}^{N} T^{-n}Q_{i_0} \cap \cdots \cap T^{-n}Q_{i_N} \text{ where } i_\ell = 1, \ldots, k, \ell = 0, \ldots, N.
\]
which plays crucial role in the construction of the measure-theoretic entropy of a dynamical system.

### 12.7 Measure-theoretic entropy

The entropy of a partition \(Q\) is defined as
\[
H(Q) = - \sum_{m=1}^{k} \mu(Q_m) \log \mu(Q_m).
\]

The measure-theoretic entropy of a dynamical system \((X, B, T, \mu)\) with respect to a partition \(Q = \{Q_1, \ldots, Q_k\}\) is then defined as
\[
h_\mu(T, Q) = \lim_{N \to \infty} \frac{1}{N} H \left( \bigvee_{n=0}^{N} T^{-n}Q \right).
\]

Finally, the **Kolmogorov–Sinai** or **metric** or **measure-theoretic entropy** of a dynamical system \((X, B, T, \mu)\) is defined as
\[
h_\mu(T) = \sup_Q h_\mu(T, Q).
\]
where the supremum is taken over all finite measurable partitions. A theorem of Yakov G. Sinai in 1959 shows that the supremum is actually obtained on partitions that are generators. Thus, for example, the entropy of the Bernoulli process is log 2, since almost every real number has a unique binary expansion. That is, one may partition the unit interval into the intervals \([0, 1/2]\) and \([1/2, 1]\). Every real number \(x\) is either less than 1/2 or not; and likewise so is the fractional part of \(2^n x\).

If the space \(X\) is compact and endowed with a topology, or is a metric space, then the topological entropy may also be defined.
12.8 See also

- Krylov–Bogolyubov theorem on the existence of invariant measures
- Poincaré recurrence theorem

12.9 References


12.10 Examples

Chapter 13

List of Feynman diagrams

This is a list of common Feynman diagrams.
Chapter 14

Canonical quantization

In physics, canonical quantization is a procedure for quantizing a classical theory, while attempting to preserve the formal structure, such as symmetries, of the classical theory, to the greatest extent possible.

Historically, this was not quite Werner Heisenberg’s route to obtaining quantum mechanics, but Paul Dirac introduced it in his 1926 doctoral thesis, the “method of classical analogy” for quantization,[1] and detailed it in his classic text.[2] The word canonical arises from the Hamiltonian approach to classical mechanics, in which a system’s dynamics is generated via canonical Poisson brackets, a structure which is only partially preserved in canonical quantization.

This method was further used in the context of quantum field theory by Paul Dirac, in his construction of quantum electrodynamics. In the field theory context, it is also called second quantization, in contrast to the semi-classical first quantization for single particles.

14.1 History

Quantum physics first dealt only with the quantization of the motion of particles, leaving the electromagnetic field classical, hence the name quantum mechanics.[3] Later the electromagnetic field was also quantized, and even the particles themselves were represented through quantized fields, resulting in the development of quantum electrodynamics (QED) and quantum field theory in general.[4] Thus, by convention, the original form of particle quantum mechanics is denoted first quantization, while quantum field theory is formulated in the language of second quantization.

14.2 First quantization

Main article: First quantization

14.2.1 Single particle systems

The following exposition is based on Dirac’s treatise on quantum mechanics.[2] In the classical mechanics of a particle, there are dynamic variables which are called coordinates (x) and momenta (p). These specify the state of a classical system. The canonical structure (also known as the symplectic structure) of classical mechanics consists of Poisson brackets between these variables, such as \( \{x, p\} = 1 \). All transformations of variables which preserve these brackets are allowed as canonical transformations in classical mechanics. Motion itself is such a canonical transformation.

By contrast, in quantum mechanics, all significant features of a particle are contained in a state \( |\psi\rangle \), called quantum state. Observables are represented by operators acting on a Hilbert space of such quantum states. The (eigen)value of an operator acting on one of its eigenstates represents the value of a measurement on the particle thus represented. For example, the energy is read off by the Hamiltonian operator \( \hat{H} \) acting on a state \( |\psi_n\rangle \), yielding

\[
\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle
\]

where \( E_n \) is the characteristic energy associated to this \( |\psi_n\rangle \) eigenstate.

Any state could be represented as a linear combination of eigenstates of energy; for example,

\[
|\psi\rangle = \sum_{n=0}^{\infty} a_n|\psi_n\rangle
\]

where \( a_n \) are constant coefficients.

As in classical mechanics, all dynamical operators can be represented by functions of the position and momentum ones, \( \hat{X} \) and \( \hat{P} \), respectively. The connection between this representation and the more usual wavefunction representation is given by the eigenstate of the position operator \( \hat{X} \) representing a particle at position \( x \), which is denoted by an element \( |x\rangle \) in the Hilbert space, and which satisfies \( \hat{X}|x\rangle = x|x\rangle \). Then, \( \psi(x) = (x|\psi\rangle \).
Likewise, the eigenstates \(|p\rangle\) of the momentum operator \(\hat{P}\) specify the momentum representation: \(\psi(p) = \langle p|\psi\rangle\).

The central relation between these operators is a quantum analog of the above Poisson bracket of classical mechanics, the canonical commutation relation,

\[ [\hat{X}, \hat{P}] = \hat{X}\hat{P} - \hat{P}\hat{X} = i\hbar \]

This relation encodes (and formally leads to) the uncertainty principle, in the form \(\Delta x \Delta p \geq \hbar/2\). This algebraic structure may be thus considered as the quantum analog of the canonical structure of classical mechanics.

### 14.2.2 Many-particle systems

When turning to \(N\)-particle systems, i.e., systems containing \(N\) identical particles (particles characterized by the same quantum numbers such as mass, charge and spin), it is necessary to extend the single-particle state function \(\psi(r)\) to the \(N\)-particle state function \(\psi(r_1, r_2, \ldots, r_N)\). A fundamental difference between classical and quantum mechanics concerns the concept of indistinguishability of identical particles. Only two species of particles are thus possible in quantum physics, the so-called bosons and fermions which obey the rules:

\[
\begin{align*}
\psi(r_1, \ldots, r_j, \ldots, r_k, \ldots, r_N) \\
+ \psi(r_1, \ldots, r_k, \ldots, r_j, \ldots, r_N) & \quad \text{(bosons),} \\
- \psi(r_1, \ldots, r_k, \ldots, r_j, \ldots, r_N) & \quad \text{(fermions).}
\end{align*}
\]

Where we have interchanged two coordinates \((r_j, r_k)\) of the state function. The usual wave function is obtained using the slater determinant and the identical particles theory. Using this basis, it is possible to solve various many-particle problems.

### 14.3 Issues and limitations

Dirac’s book\(^2\) details his popular rule of supplanting Poisson brackets by commutators:

\[
\{x^i, p^j\} + \frac{1}{i\hbar}\{\{p^j, x^i\}, \{x^i, p^j\}\} = 0
\]

\[
\frac{1}{\pi^2} [\hat{x}^3, \hat{p}^3] + \frac{1}{12\pi^2} \left[ \frac{1}{3!} [\hat{p}^3, \hat{x}^3], \frac{1}{3!} [\hat{x}^3, \hat{p}^3] \right] = -3\hbar^2.
\]

The right-hand-side “anomaly” term \(-3\hbar^2\) is not predicted by application of the above naive quantization rule. In order to make this procedure more rigorous, one might hope to take an axiomatic approach to the problem. If \(Q\) represents the quantization map that acts on functions \(f\) in classical phase space, then the following properties are usually considered desirable:\(^6\)

1. \(Q_x \psi = x\psi\) and \(Q_p \psi = -i\hbar \partial_x \psi\) (elementary position/momentum operators)
2. \(f \mapsto Q_f\) is a linear map
3. \([Q_f, Q_g] = i\hbar Q_{\{f,g\}}\) (Poisson bracket)
4. \(Q_{gf} = g(Q_f)\) (von Neumann rule).

However, not only are these four properties mutually inconsistent, any three of them is also inconsistent!\(^7\) As it turns out, the only pairs of these properties that lead to self-consistent, nontrivial solutions are 2+3 and possibly 1+3 or 1+4. Accepting properties 1+2 along with a weaker condition that 3 be true only asymptotically in the limit \(\hbar \to 0\) (see Moyal bracket) is deformation quantization, and some extraneous information must be provided, as in the standard theories utilized in most of physics. Accepting properties 1+2+3 but restricting the space of quantizable observables to exclude terms such as the cubic ones in the above example amounts to geometric quantization.

### 14.4 Second quantization: field theory

Quantum mechanics was successful at describing non-relativistic systems with fixed numbers of particles, but a new framework was needed to describe systems in which particles can be created or destroyed, for example, the electromagnetic field, considered as a collection of photons. It was eventually realized that special relativity was inconsistent with single-particle quantum mechanics, so that all particles are now described relativistically by quantum fields.

When the canonical quantization procedure is applied to a field, such as the electromagnetic field, the classical field variables become quantum operators. Thus, the normal modes comprising the amplitude of the field become quantized, and the quanta are identified with individual particles or excitations. For example, the quanta of the
electromagnetic field are identified with photons. Unlike first quantization, conventional second quantization is completely unambiguous, in effect a functor.

Historically, quantizing the classical theory of a single particle gave rise to a wavefunction. The classical equations of motion of a field are typically identical in form to the (quantum) equations for the wave-function of one of its quanta. For example, the Klein–Gordon equation is the classical equation of motion for a free scalar field, but also the quantum equation for a scalar particle wavefunction. This meant that quantizing a field appeared to be similar to quantizing a theory that was already quantized, leading to the fanciful term second quantization in the early literature, which is still used to describe field quantization, even though the modern interpretation detailed is different.

One drawback to canonical quantization for a relativistic field is that by relying on the Hamiltonian to determine time dependence, relativistic invariance is no longer manifest. Thus it is necessary to check that relativistic invariance is not lost. Alternatively, the Feynman integral approach is available for quantizing relativistic fields, and is manifestly invariant. For non-relativistic field theories, such as those used in condensed matter physics, Lorentz invariance is not an issue.

14.4. SECOND QUANTIZATION: FIELD THEORY

Quantum mechanically, the variables of a field (such as the field’s amplitude at a given point) are represented by operators on a Hilbert space. In general, all observables are constructed as operators on the Hilbert space, and the time-evolution of the operators is governed by the Hamiltonian, which must be a positive operator. A state $|0\rangle$ annihilated by the Hamiltonian must be identified as the vacuum state, which is the basis for building all other states. In a non-interacting (free) field theory, the vacuum is normally identified as a state containing zero particles. In a theory with interacting particles, identifying the vacuum is more subtle, due to vacuum polarization, which implies that the physical vacuum in quantum field theory is never really empty. For further elaboration, see the articles on quantum mechanical vacuum and the vacuum of quantum chromodynamics. The details of the canonical quantization depend on the field being quantized, and whether it is free or interacting.

### 14.4.1 Field operators

A scalar field theory provides a good example of the canonical quantization procedure. Classically, a scalar field is a collection of an infinity of oscillator normal modes. For simplicity, the quantization can be carried out in a 1+1 dimensional space-time $\mathbb{R} \times S_1$, in which the spatial direction is compactified to a circle of circumference $2\pi$, rendering the momenta discrete. The classical Lagrangian density is then

$$\mathcal{L}(\phi) = \frac{1}{2} (\partial_t \phi)^2 - \frac{1}{2} (\partial_x \phi)^2 - \frac{1}{2} m^2 \phi^2 - V(\phi),$$

where $V(q)$ is a potential term, often taken to be a polynomial or monomial of degree 3 or higher. The action functional is

$$S(\phi) = \int \mathcal{L}(\phi)dxdt = \int L(\phi, \partial_t \phi) dt$$

The canonical momentum obtained via the Legendre transform using the action $L$ is $\pi = \partial_t \phi$, and the classical Hamiltonian is found to be

$$H(\phi, \pi) = \int dx \left[ \frac{1}{2} \pi^2 + \frac{1}{2} (\partial_x \phi)^2 + \frac{1}{2} m^2 \phi^2 + V(\phi) \right].$$

Canonical quantization treats the variables $\phi(x)$ and $\pi(x)$ as operators with canonical commutation relations at time $t = 0$, given by

$$[\phi(x), \phi(y)] = 0, \quad [\pi(x), \pi(y)] = 0, \quad [\phi(x), \pi(y)] = i\hbar \delta(x-y).$$

Operators constructed from $\phi$ and $\pi$ can then formally be defined at other times via the time-evolution generated by the Hamiltonian:

$$\mathcal{O}(t) = e^{iHt} \mathcal{O} e^{-iHt}.$$
\[ \phi_{-k} = \phi_k^\dagger, \quad \pi_{-k} = \pi_k^\dagger \]

The classical Hamiltonian may be expanded in Fourier modes as

\[
H = \frac{1}{2} \sum_{k=-\infty}^{\infty} \left[ \pi_k \pi_k^\dagger + \omega_k^2 \phi_k \phi_k^\dagger \right],
\]

where \( \omega_k = \sqrt{k^2 + m^2} \).

This Hamiltonian is thus recognizable as an infinite sum of classical normal mode oscillator excitations \( q_k \), each one of which is quantized in the standard manner, so the free quantum Hamiltonian looks identical. It is the \( q_k \)'s that have become operators obeying the standard commutation relations, \([q_k, \pi_k'] = [q_k', \pi_k] = i\hbar\), with all others vanishing. The collective Hilbert space of all these oscillators is thus constructed using creation and annihilation operators constructed from these modes,

\[
a_k = \frac{1}{\sqrt{2\hbar \omega_k}} (\omega_k \phi_k + i \pi_k), \quad a_k^\dagger = \frac{1}{\sqrt{2\hbar \omega_k}} (\omega_k \phi_k^\dagger - i \pi_k),
\]

for which \([a_k, a_k^\dagger] = 1\) for all \( k \), with all other commutators vanishing.

The vacuum \( |0\rangle \) is taken to be annihilated by all of the \( a_k \), and \( \mathcal{H} \) is the Hilbert space constructed by applying any combination of the infinite collection of creation operators \( a_k^\dagger \) to \( |0\rangle \). This Hilbert space is called Fock space. For each \( k \), this construction is identical to a quantum harmonic oscillator. The quantum field is an infinite array of quantum oscillators. The quantum Hamiltonian then amounts to

\[
H = \sum_{k=-\infty}^{\infty} \hbar \omega_k a_k^\dagger a_k = \sum_{k=-\infty}^{\infty} \hbar \omega_k N_k
\]

where \( N_k \) may be interpreted as the number operator giving the number of particles in a state with momentum \( k \).

This Hamiltonian differs from the previous expression by the subtraction of the zero-point energy \( \hbar \omega_k / 2 \) of each harmonic oscillator. This satisfies the condition that \( H \) must annihilate the vacuum, without affecting the time-evolution of operators via the above exponentiation operation. This subtraction of the zero-point energy may be considered to be a resolution of the quantum operator ordering ambiguity, since it is equivalent to requiring that all creation operators appear to the left of annihilation operators in the expansion of the Hamiltonian. This procedure is known as Wick ordering or normal ordering.

**Other fields**

All other fields can be quantized by a generalization of this procedure. Vector or tensor fields simply have more components, and independent creation and destruction operators must be introduced for each independent component. If a field has any internal symmetry, then creation and destruction operators must be introduced for each component of the field related to this symmetry as well. If there is a gauge symmetry, then the number of independent components of the field must be carefully analyzed to avoid over-counting equivalent configurations, and gauge-fixing may be applied if needed.

It turns out that commutation relations are useful only for quantizing bosons, for which the occupancy number of any state is unlimited. To quantize fermions, which satisfy the Pauli exclusion principle, anti-commutators are needed. These are defined by \([A,B] = AB + BA\).

When quantizing fermions, the fields are expanded in creation and annihilation operators, \( \theta k^\dagger \), \( \theta k \), which satisfy

\[
\{ \theta_k, \theta_k^\dagger \} = \delta_{kl}, \quad \{ \theta_k, \theta_l \} = 0, \quad \{ \theta_k^\dagger, \theta_l^\dagger \} = 0.
\]

The states are constructed on a vacuum \( |0\rangle \) annihilated by the \( \theta k \), and the Fock space is built by applying all products of creation operators \( \theta k^\dagger \) to \( |0\rangle \). Pauli’s exclusion principle is satisfied, because \((\theta_k^\dagger)^2 |0\rangle = 0\), by virtue of the anti-commutation relations.

**14.4.2 Condensates**

The construction of the scalar field states above assumed that the potential was minimized at \( q = 0 \), so that the vacuum minimizing the Hamiltonian satisfies \( \delta \mathcal{H} \mid q \neq 0 \), indicating that the vacuum expectation value (VEV) of the field is zero. In cases involving spontaneous symmetry breaking, it is possible to have a non-zero VEV, because the potential is minimized for a value \( q = v \). This occurs for example, if \( V(q) = gq^4 + m^2 q^2 \), for which the minimum energy is found at \( v = \pm m/\sqrt{g} \). The value of \( v \) in one of these vacua may be considered as condensate of the field \( \phi \). Canonical quantization then can be carried out for the shifted field \( \phi(x, t) - v \), and particle states with respect to the shifted vacuum are defined by quantizing the shifted field. This construction is utilized in the Higgs mechanism in the standard model of particle physics.

**14.5 Mathematical quantization**

The classical theory is described using a spacelike foliation of spacetime with the state at each slice being described by an element of a symplectic manifold with the time evolution given by the symplectomorphism generated by a Hamiltonian function over the symplectic
manifold. The quantum algebra of “operators” is an ħ-deformation of the algebra of smooth functions over the symplectic space such that the leading term in the Taylor expansion over ħ of the commutator \([A, B]\) expressed in the phase space formulation is \(i\hbar \{A, B\}\). (Here, the curly braces denote the Poisson bracket. The subleading terms are all encoded in the Moyal bracket, the suitable quantum deformation of the Poisson bracket.) In general, for the quantities (observables) involved, and providing the arguments of such brackets, ħ-deformations are highly nonunique—quantization is an “art”, and is specified by the physical context. (Two different quantum systems may represent two different, inequivalent, deformations of the same classical limit, \(\hbar \to 0\).)

Now, one looks for unitary representations of this quantum algebra. With respect to such a unitary representation, a symplectomorphism in the classical theory would now deform to a (metaplectic) unitary transformation. In particular, the time evolution symplectomorphism generated by the classical Hamiltonian deforms to a unitary transformation generated by the corresponding quantum Hamiltonian.

A further generalization is to consider a Poisson manifold instead of a symplectic space for the classical theory and perform an ħ-deformation of the corresponding Poisson algebra or even Poisson supermanifolds.

14.6 See also
- Correspondence principle
- Creation and annihilation operators
- Dirac bracket
- Moyal bracket
- Weyl quantization
- Geometric quantization

14.7 References


14.7.1 Historical References

14.7.2 General Technical References

14.8 External links

- What is “Relativistic Canonical Quantization”?
- Pedagogic Aides to Quantum Field Theory Click on the links for Chaps. 1 and 2 at this site to find an extensive, simplified introduction to second quantization. See Sect. 1.5.2 in Chap. 1. See Sect. 2.7 and the chapter summary in Chap. 2.
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