Mathematical Modelling

Lecture 5

Hurtling through space

Newtonian mechanics

- Newtonian mechanics addresses systems of mass points. A mass point is a single point moving in space that has a finite mass m attached to it.

- Newton's law:

$$\text{mass} \times \text{acceleration} = \text{force}$$

- Newton's apple: (a mass point with mass m and vertical position $z(t)$ at time t). The force is $-mg$:

$$m\ddot{z} = -mg \iff \ddot{z} = -g$$

- Second order ODE, solving IVP requires two initial conditions:

$$z(t) = z(0) + \dot{z}(0)t - \frac{g}{2}t^2$$

- The state of the system is the collection of variables that completely specifies it at a moment in time

$$\text{state} = \{\text{position}, \text{velocity}\} = \{z, \dot{z}\}$$

- If the motion is well-posed then $\text{state}(0) \rightarrow \text{state}(t)$ (determinism).

Mechanical systems

More generally, a motion in $\mathbb{R}^n$ is a differential mapping

$$x(t) : I \to \mathbb{R}^n$$

where I is an interval on the real axis. The first derivative of the motion $\dot{x}(t) = dx/dt$ is the velocity vector. The second derivative of the motion $\ddot{x}(t) = d^2x/dt^2$ is the acceleration vector.

A mechanical system of n points moving in three-dimensional euclidean space is defined as follows: the graph (t, x) of a motion is a curve in $\mathbb{R} \times \mathbb{R}^3$ A motion of n points gives n curves. The direct product of n copies of $\mathbb{R}^3$ is called the configuration space of the system of n points, i.e. $\mathbb{R}^N, \ N = 3n$

We say the system has N degrees of freedom. The phase space is dimension 2N.

Newton's principle of determinacy: the initial state of a mechanical system (the totality of the positions and velocities of its points at some moment in time) uniquely determines all of its motion.

Newtonian mechanics

- Energy conservation: Multiply by the velocity and manipulate

$$\ddot{z} = -g$$

$$\dot{z}\ddot{z} + g\dot{z} = 0 \iff \frac{d}{dt}\left(\frac{\dot{z}^2}{2} + gz\right) = 0$$

- The invariant quantity is the energy functional (actually times m)

$$H(z, \dot{z}) = \frac{\dot{z}^2}{2} + gz = \text{const} = E$$

- E is determined from the initial condition
- First term is the kinetic energy, second term the potential energy.
- Phase space: the space spanned by the state coordinates $(z, \dot{z})$
  - Every state of the system corresponds to a point (space of all possible states)
  - Solutions define nonintersecting trajectories (curves) in phase space
  - Trajectories coincide with contours of constant H.
- Plotting the contours of H we can produce the solutions without solving the ODE (but not their parameterization in time).

Galilean invariance

- Galilean space: $\mathbb{R} \times \mathbb{R}^3$ equipped with a distance function $|\cdot|$ for points in $\mathbb{R}^3$.

- A Galilean group is a group of transformations g of a Galilean space which preserve its structure:

  - Uniform motion with a velocity v

    $$g(t,x) = (t, x + vt), \quad t \in \mathbb{R},\ x, t \in \mathbb{R}^3$$

  - Translation of the origin

    $$g(t,x) = (t + s, x + y)$$

  - Rotation of the coordinate axes

    $$g(t,x) = (t, Gx)$$

where $G : \mathbb{R}^3 \to \mathbb{R}^3$ is an orthogonal matrix. Every Galilean transformation can be written as a composition of these.

Galilean invariance

- Newton's law

$$m\ddot{x} = F(x, \dot{x}, t)$$

- If the motion is Galilean invariant (inertial coordinate system):
  - Time translation: $x = \phi(t)$ a solution, then $x = \phi(t+s)$ is too, $\forall s$.

    $$m\ddot{x} = F(x, \dot{x})$$

  - Space translations: $x_i = \phi_i(t),\ i = 1, \ldots, n$ are motions of an n-point system, then so are $x_i = \phi_i(t) + r,\ i = 1, \ldots, n,\ \forall r \in \mathbb{R}^3$

    $$\ddot{x}_i = f_i(\{x_j - x_k\}, \{\dot{x}_j - \dot{x}_k\}), \quad i, j, k = 1, \ldots, n$$

  - Rotations in $\mathbb{R}^3$: if $x_i = \phi_i(t),\ i = 1, \ldots, n$ are motions satisfying Newton, and G is a 3x3 orthogonal matrix, then $x_i(t) = G\phi_i(t)$ is also a solution (no preferred direction)

$$f_i(\{Gx_j - Gx_k\}, \{G\dot{x}_j - G\dot{x}_k\}) = Gf_i(\{x_j - x_k\}, \{\dot{x}_j - \dot{x}_k\}), \quad i, j, k = 1, \ldots, n$$

Conservative forces

- Newton's law:

$$m\ddot{x} = F(x, \dot{x})$$

- F is a conservative force if it is the gradient of a potential function U(x)

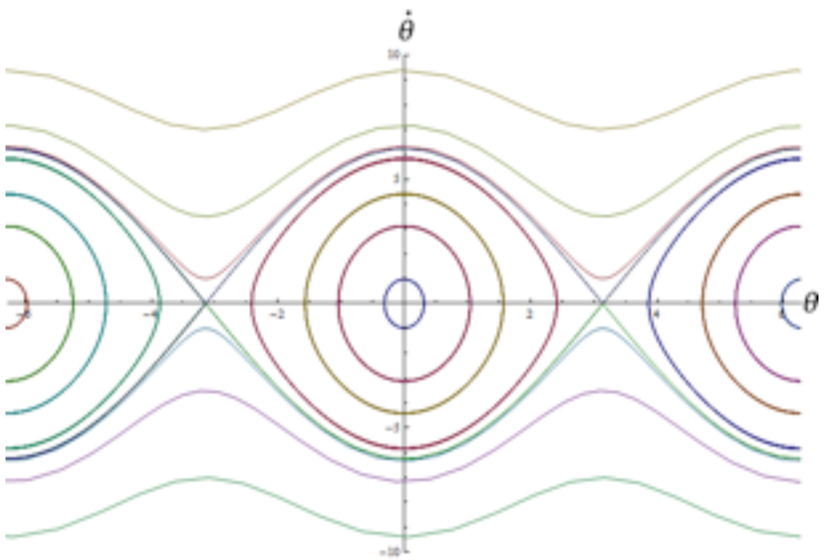
$$F = -\nabla U(x)$$

- Example 1. The gravitational potential $U = mgz \quad H = \frac{m\dot{z}^2}{2} + mgz$
- Example 2. Projectile problem $m\ddot{x} = -\dfrac{mgR^2}{(R+x)^2}$

$$U = \frac{mgR^2}{R+x} \qquad H = \frac{m|\dot{x}|^2}{2} + U$$

- Example 3. Pendulum $\ddot{\theta} + \dfrac{g}{\ell}\sin\theta = 0$

$$U = -\frac{g}{\ell}\cos\theta$$



n-body problems

- Example 4. Consider n point masses in $\mathbb{R}^3$

$$m_i \ddot{x}_i(t) = -\frac{\partial U}{\partial x_i}, \quad i = 1, \ldots, n$$

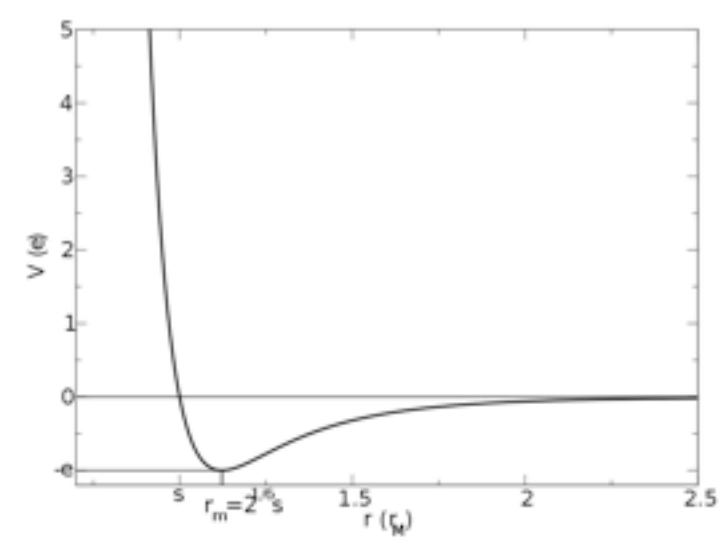
- Typically, the potential U is a sum of pair-potentials $\phi(r)$

$$U = \sum_i \sum_{j>i} m_i m_j \phi(|x_i - x_j|^2)$$

- Note that this system is Galilean invariant.

- Examples: cellestial mechanics (gravitational potential), classical molecular systems (Lennard-Jones potential):

$$\phi(r) = 4\varepsilon \left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6$$



Calculus of Variations

- Until now, we have seen the interpretation of mechanics as an initial value problem, where the motion q(t) is the solution taking the initial condition from t=0 to t=T.

- An alternative view point looks at the entire path, defining q(t) on the entire interval [0,T] as the solution to an integral equation.

- Consider a *smooth* function $y(x), \; x \in [a,b]$ and an integral

$$J[y(x)] = \int_a^b F(y, y', x)\, dx$$

- Derivatives of F with respect to its arguments: $\dfrac{\partial F}{\partial y}, \quad \dfrac{\partial F}{\partial y'}, \quad \dfrac{\partial F}{\partial x}$

$$F = x^2 y + (y')^2 \quad \Rightarrow \quad \frac{\partial F}{\partial y} = x^2, \quad \frac{\partial F}{\partial y'} = 2y', \quad \frac{\partial F}{\partial x} = 2xy, \quad \frac{\partial^2 F}{\partial x \partial y} = 2x$$

- Functional J depends on the entire function y, denoted by square brackets. Example: norms on function spaces.

Calculus of Variations

- Consider a *smooth* function $y(x), \; x \in [a,b]$ and an integral

$$J[y(x)] = \int_a^b F(y, y', x)\, dx$$

- Calculus of variations is concerned with the change of J due to small changes in y(x)

$$y(x) \to y(x) + \delta y(x)$$

- The variation $\delta y(x)$ is a smooth function that is small in the sense

$$\|\delta y(x)\|_\infty \ll 1 \text{ and } \|\delta y'\|_\infty \ll 1 \qquad \delta y' = \frac{d}{dx}\delta y$$

- Change in J (the first variation) can be computed via Taylor expansion

$$J[y + \delta y] - J[y] = \int_a^b \left(F(y + \delta y, y' + \delta y', x) - F(y, y', x)\right)\, dx$$

$$= \int_a^b \left(\delta y \frac{\partial F}{\partial y}(y, y', x) + \delta y' \frac{\partial F}{\partial y'}(y, y', x) \right) dx + o(\delta y^2, \delta y'^2)$$

$$\delta J = \int_a^b \left[\frac{\partial F}{\partial y} - \frac{\partial}{\partial x}\left(\frac{\partial F}{\partial y'} \right) \right] \delta y\, dx + \frac{\partial F}{\partial y'} \delta y \Big|_a^b$$

Calculus of Variations

- Consider a *smooth* function $y(x),\ x \in [a,b]$ and an integral

$$J[y(x)] = \int_a^b F(y, y', x)\, dx$$

- First variation:

$$\delta J = \int_a^b \left[\frac{\partial F}{\partial y} - \frac{\partial}{\partial x}\left(\frac{\partial F}{\partial y'} \right) \right] \delta y \, dx + \frac{\partial F}{\partial y'} \delta y \bigg|_a^b$$

- An extremal is a function $y(x)$ for which the first variation vanishes. In particular, in the interior it must satisfy the Euler-Lagrange equation (EL)

$$\text{EL:} \quad \frac{d}{dx}\left(\frac{\partial F}{\partial y'} \right) = \frac{\partial F}{\partial y}$$

- Boundary conditions: $y(a),\ y(b)$ fixed $\Rightarrow \delta y(a) = \delta y(b) = 0$

$$y(b) \text{ not fixed } \Rightarrow \frac{\partial F}{\partial y'}(b) = 0$$

Calculus of Variations

- Example: shortest distance between two points (x_a, y_a) and (x_b, y_b).

$$J = \int_a^b ds = \int_a^b \sqrt{dx^2 + dy^2} = \int_{x_a}^{x_b} \sqrt{1 + y'^2}\, dx$$

- Euler-Lagrange equation is

$$\frac{d}{dx}\left(\frac{\partial F}{\partial y'}\right) = 0 \quad \Rightarrow \quad \frac{\partial F}{\partial y'} = \frac{y'}{\sqrt{1 + y'^2}} = \text{const.}$$

- Hence the extremal is a straight line through the two endpoints.

- In a variant we do not specify $y(x_b) = y_b$. Then the natural boundary condition comes into play $y'(x_b) = 0$, and the extremal is a straight line of zero slope.

Symmetries and conservation laws

- A conservation law is a function $G(y, y', x)$ that is constant along extremals of the functional. For y(x) a solution to the EL equations:

$$\frac{dG}{dx} = \frac{\partial G}{\partial x} + \frac{\partial G}{\partial y} y' + \frac{\partial G}{\partial y'} y'' = 0$$

- It turns out that many conservation laws can be related to continuous symmetries of J. For instance, in the previous example, J depended only on y', not explicitly on x and y. This led to the conservation law

$$\frac{d}{dx}\left(\frac{\partial F}{\partial y'}\right) = 0$$

- A translational symmetry in x or y yields a conservation law. A symmetry in the dependent variable y means $F = F(y', x)$ and hence for $G_y \equiv \partial F / \partial y'$, using the EL equations:

$$\frac{dG_y}{dx} = \frac{d}{dx}\left(\frac{\partial F}{\partial y'}\right) = \frac{\partial F}{\partial y} = 0$$

- Similarly for $F = F(y, y')$ we have conservation of $G_x = y' \partial F / \partial y' - F$

Action principle

- Returning to Newton's apple, we define the action functional

$$S[z(t)] = \int_0^T L(z, \dot{z})\, dt = \int_0^T (K - U)\, dt = \int_0^T \left(m\frac{\dot{z}^2}{2} - mgz \right) dt$$

- The quantity L is referred to as the Lagrangian, the difference between kinetic and potential energies.

- The action principle: Newton's law is the Euler-Lagrange equation for an extremal of the action integral relative to all trajectories that have a fixed initial point z(0) and a fixed terminal point z(T):

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{z}} = \frac{\partial L}{\partial z}, \qquad \frac{\partial L}{\partial z} = -mg, \;\; \frac{\partial L}{\partial \dot{z}} = m\dot{z} \quad \Rightarrow \quad \ddot{z} = -g$$

- As opposed to the IVP approach, here need to specify the boundary data (BVP)

- Since the Lagrangian does not explicitly depend on t, there is a conservation law (energy)

$$G_t = \dot{z}\frac{\partial L}{\partial \dot{z}} - L = m\frac{\dot{z}^2}{2} + mgz = H(z, \dot{z})$$

Action principle

- The Euler-Lagrange equations generalize easily to functionals that depend on more than one function $F(x_1, \ldots, x_N, x'_1, \ldots, x'_N, t)$

$$\frac{d}{dt}\left(\frac{\partial F}{\partial x'_n}\right) = \frac{\partial F}{\partial x_n}, \quad n = 1, \ldots, N$$

- The action principle is still defined as the difference between kinetic and potential energies:

$$S[x(t)] = \int_0^T L(x, \dot{x})\, dt = \int_0^T (K - U)\, dt = \int_0^T \frac{|\dot{x}|^2}{2} - U(x)\, dt = 0$$

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} = \frac{\partial L}{\partial x} \quad \Rightarrow \quad \ddot{x} + \nabla U(x) = 0$$

Coordinate invariance

- The Euler-Lagrange equations are invariant under arbitrary changes of coordinates. If x satisfies the EL equations and $x = f(X)$ then X satisfies the EL equations for the action principle with Lagrangian

$$\tilde{L}(X, \dot{X}, t) = L(f(X), f'(X)\dot{X}, t)$$

- To see this substitute

$$\frac{\partial \tilde{L}}{\partial X} = \frac{\partial L}{\partial x} f(X) + \frac{\partial L}{\partial \dot{x}} f''(X)\dot{X}, \qquad \frac{\partial \tilde{L}}{\partial \dot{X}} = \frac{\partial L}{\partial \dot{x}} f'(X)$$

$$\frac{d}{dt}\left(\frac{\partial \tilde{L}}{\partial \dot{X}}\right) = \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) f' + \frac{\partial L}{\partial \dot{x}} f''\dot{X} = \frac{\partial L}{\partial x} f' + \frac{\partial L}{\partial \dot{x}} f''\dot{X} = \frac{\partial \tilde{L}}{\partial X}$$

- The same does not hold for Newton's equations.