Hamiltonian

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1 Canonical system and Hamiltonian

In this section, we bring Euler equations to the standard form using a modified form of Lagrangian.

1.1 canonical form of Euler equations

The Euler equations for a vector minimizer $u = (u_1, \ldots, u_N)$ is a system of N second-rank differential equations:

$$\frac{d}{dx}\frac{\partial L}{\partial u_i'} - \frac{\partial L}{\partial u_i} = 0, \quad i = 1, \ldots, N \tag{1}$$

with boundary conditions

$$\Theta_a(u, u')|_{x=a} = 0, \quad \Theta_b(u, u')|_{x=b} = 0 \tag{2}$$

where Θ_a and Θ_b are N-dimensional vector functions.

The structure of this system can be simplified and unified if it is rewritten as a system of $2N$ first-order differential equations in a standard form

$$z_i = f_i(z_1, \ldots, z_{2N}), \quad i = 1, \ldots, 2N$$

instead of N second-order equations. This system can be obtained from (**??**) if new variables p_i are introduced,

$$p_i(x) = \frac{\partial L(x, u, u')}{\partial u_i'}, \quad i = 1, \ldots, N \tag{3}$$

In mechanics, $p = (p_1, \ldots, p_N)$ is called the vector of *impulse*. The Euler equation takes the form

$$p' = \frac{\partial L(x, u, u')}{\partial u} = f(x, u, u'), \tag{4}$$

where f is a vector-valued function of x, u, u'. The system (**??**), (**??**) becomes symmetric with respect to p and u if we algebraically solve (**??**) for u' and find:

$$u' = \phi(x, u, p). \tag{5}$$

Then, substitute this expression into (**??**) and obtain:

$$p' = f(x, u, \phi(x, u, p)) = \psi(x, u, p) \tag{6}$$

where ψ is a function of the variables u and p but not of their derivatives. Equations (**??**), (**??**) form the canonical system of $2N$ equations for $2N$ unknown functions u_i, p_j, $i, j = 1, \ldots, N$.

The boundary conditions (**??**) are rewritten in terms of u and p excluding u' by (**??**); they take the form

$$\Theta_a(u, \phi(a, u, p),)|_{x=a} = \theta_a(u, p) = 0, \quad \Phi_b(u, u')|_{x=b} = \theta_b(u, p) = 0 \tag{7}$$

where θ_a and θ_b are N-dimensional vector functions.

In summary, system (**??**), (**??**) transfers Euler equation to the canonical form (or Cauchy form)

$$\begin{array}{l} u' = \phi(x, u, p) \\ p' = \psi(x, u, p) \end{array} \tag{8}$$

$$\theta_a(u, p) = 0, \quad \theta_b(u, p) = 0. \tag{9}$$

The solution to the canonical system is entirely determined by the algebraic vector functions ϕ, ψ in the right-hand side which do not contain derivatives, and by the boundary conditions. Notice that functions u and p are differentiable.

Example 1.1 (Quadratic Lagrangian) Assume that Lagrangian L and boundary conditions are:

$$L = \frac{1}{2}a(x)u'^2 + \frac{1}{2}b(x)u^2, \quad u(x_0) = u_0, \quad \frac{\partial L}{\partial u'}|_{x=x_1} = 0$$

The Euler equation

$$(a\, u')' - bu = 0$$

is transformed as follows. We introduce p as in (**??**)

$$p = \frac{\partial L(x, u, u')}{\partial u'} = au'$$

and obtain the canonical system and boundary conditions

$$\begin{array}{l} u' = \frac{1}{a(x)}p \\ p' = b(x)u \\ u(x_0) = u_0, \quad p(x_1) = 0 \end{array}$$

Notice that the coefficient $a(x)$ is moved into denominator.

Canonical system for equations of Lagrangian mechanics The equations of Lagrangian mechanics correspond to stationarity of the action. The functional of action is

$$L(t,q,q') = T(q,q') - V(q), \quad T(q,q') = \frac{1}{2}(q')^T R(q) q'$$

where positively defined symmetric matrix $R(q)$ is the matrix of inertia, and $V(q)$ (potential energy) is a convex function of the N dimensional vector of generalized coordinates $q = q_1, \ldots, N$.

The vector-valued Euler equation

$$\frac{d}{dt}\frac{\partial T}{\partial q'} = \frac{\partial T}{\partial q} - \frac{\partial V}{\partial q} \tag{10}$$

is of order $2N$.

To bring the system (**??**) to canonical form, we introduce vector of impulses

$$p = \frac{\partial T}{\partial q'} = R(q)q'$$

The Euler equation becomes:

$$p' = \frac{\partial T}{\partial q} - \frac{\partial V}{\partial q}$$

Kinetic energy T is expressed through p as

$$T = \frac{1}{2}(q')^T R q' = \frac{1}{2}p^T \left(R^{-1}\right) p.$$

The first term in the right-hand side of (**??**) becomes

$$\frac{\partial T}{\partial q} = \frac{1}{2}p^T \left(\frac{dR^{-1}}{dq}\right) p$$

The canonical system becomes

$$\begin{aligned} q' &= R^{-1}p, \\ p' &= \tfrac{\partial T}{\partial q} - \tfrac{\partial V}{\partial q} = \tfrac{1}{2}p^T \left(\tfrac{dR^{-1}}{dq}\right) p - \tfrac{\partial V}{\partial q} \end{aligned}$$

Example 1.2 (Rotating mass 1) Consider a mass m attached by a spring to a fixed point; call this point the origin. The force F in the spring is the derivative of a potential $V(|r|)$, where $r = (r_1, r_2, r_3)$ is the vector of coordinates of a point, $|r| = \sqrt{r_1^2 + r_2^2 + r_3^2}$ is the distance fro the origin. The force F is computed as

$$F = \frac{dV}{dr} = \frac{dV'}{d|r|}\frac{d|r|}{dr} = \left(\frac{1}{|r|}\frac{dV}{d|r|}\right) r = \phi(|r|) r$$

where

$$\phi(|r|) = \frac{1}{|r|}\frac{dV}{d|r|}$$

The Lagrangian is

$$L = T - V = \frac{1}{2} m r'^T r' - V(|r|)$$

Euler equations are

$$(mr')' - \frac{\partial V}{\partial r} = 0 \quad \text{or } (mr')' - \phi(|r|) r = 0$$

Introducing the impulse vector $p = mr'$ and we write canonical system as

$$r' = \frac{1}{m} p, \quad p' = \phi(|r|) r \tag{11}$$

Planar motion Analyzing system (**??**), we conclude that the motion is planar. Indeed, consider vector product $z = r \times p$ and compute its time derivative:

$$\frac{dz}{dt} = \frac{d}{dt}(r \times p) = r' \times p + r \times p' = 0$$

This vector is constant because vector r' is proportional to p and p' is proportional to r, see (**??**). The constancy of z indicates that vectors $r(t)$ and $p(t)$ remain all the time perpendicular to vector z; they are moving in a plane L, that passes through the point of initial conditions $r(0) = r_0,\ p(0) = p_0$ and the origin.

In the plane L, we introduce polar coordinates ρ, θ; Potential energy depends only on ρ, $V = V(\rho)$, and kinetic energy becomes

$$T = \frac{m}{2}(\rho'^2 + \rho^2 \theta'^2) = \frac{1}{2} p^T R^{-1} p$$

where

$$p = \begin{pmatrix} p_\rho \\ p_\theta \end{pmatrix} \quad R = \begin{pmatrix} m & 0 \\ 0 & m\rho^2 \end{pmatrix}$$

The canonical system becomes

$$\dot{\rho} = \frac{1}{m} p_\rho, \tag{12}$$

$$\dot{\theta} = \frac{1}{m\rho^2} p_\theta, \tag{13}$$

$$\dot{p_\rho} = -\frac{2}{m\rho^3} p_\rho - \frac{\partial V}{\partial \rho} \tag{14}$$

$$\dot{p_\theta} = 0 \tag{15}$$

Example 1.3 (Geometrical optics) In geometrical optics, Lagrangian $F = w(y)\sqrt{1 + y'^2}$ corresponds to Euler equation

$$\frac{d}{dt}\left(\frac{w(y) y'}{\sqrt{1 + y'^2}}\right) = \frac{dw}{dy}$$

To derive the canonical system, we call

$$p = \frac{w(y)y'}{\sqrt{1+y'^2}} \tag{16}$$

The canonical system for geometric optics is

$$\begin{aligned} p' &= \frac{dw}{dy} \\ y' &= \pm\frac{p}{\sqrt{w^2-p^2}} \end{aligned}$$

The first equation is obtained by substitution of p from (**??**) into Euler equattion. The second equation is obtained when we solve (**??**) for y' as follows:

$$p^2 = \frac{w(y)^2 {y'}^2}{1+y'^2}, \quad {y'}^2 = \frac{p^2}{w^2-p^2}$$

1.2 Hamiltonian

We can rewrite the system (**??**) in a more symmetric form introducing a special potential function called *Hamiltonian.* The Hamiltonian is defined by the formula (see (**??**)):

$$H(x,u,p) = pu'(x,u,p) - L(x,u,u'(u,p))$$

or

$$H(x,u,p) = p\phi(x,u,p) - L(x,u,\phi(x,u,p)) \tag{17}$$

where u is a stationary trajectory – the solution of Euler equation.

Hamiltonian allows to write canonical system (**??**) in a remarkable symmetric form

$$p' = -\frac{\partial H}{\partial u}, \quad p' = -\frac{\partial H}{\partial u} \tag{18}$$

To show this form, compute the partial derivatives of H (**??**) : We have

$$\frac{\partial H}{\partial u} = p\frac{\partial \phi}{\partial u} - \frac{\partial L}{\partial u} - \frac{\partial L}{\partial \phi}\frac{\partial \phi}{\partial u}$$

By the definition (**??**) of p, $p = \frac{\partial L}{\partial u'} = \frac{\partial L}{\partial \phi}$, hence the first and third term in the right-hand side cancel. By virtue of the Euler equation (**??**), the remaining term $\frac{\partial L}{\partial u}$ is equal to p' and we obtain the first equation in (**??**)

Next, compute $\frac{\partial H}{\partial p}$. We have

$$\frac{\partial H}{\partial p} = \phi + p\frac{\partial \phi}{\partial p} - \frac{\partial L}{\partial \phi}\frac{\partial \phi}{\partial p}$$

By definition of p, the second and the third term in the right-hand side cancel, and by definition of ϕ ($\phi = u'$) we obtain the second equation in (**??**)

The right-hand side functions in the canonical system (**??**) are expressed through the partial derivatives of a single function potential $H(u,p)$.

Hamiltonian for Lagrangian mechanics In Lagrangian mechanics, the Hamiltonian H is equal to the sum of kinetic and potential energy or to the whole energy, $H = T + V$ where q' is expressed through p, and q, $q' = R(q)^{-1}p$

$$H(q,p) = \frac{1}{2}p^T R^{-1} p + V$$

Indeed, kinetic energy is a second degree homogeneous function of p, which implies

$$p^T \frac{\partial T}{\partial p} = p^T R(q) p = 2T$$

and

$$H = p^T \frac{\partial T}{\partial p} - L = 2T - (T - V) = T + V$$

Hamiltonian and canonical equations in Example (**??**) are

$$L = \frac{1}{2}(a(x)u'^2 + b(x)u^2) = \frac{1}{2}\left(\frac{1}{a(x)}p^2 + b(x)u^2\right)$$

then the Hamiltonian is

$$H = p\left(\frac{p}{a}\right) - L = \frac{1}{2}\left(\frac{1}{a(x)}p^2 - b(x)u^2\right)$$

and the canonical system is

$$\frac{\partial H}{\partial u} = -b(x)u = -p', \quad \frac{\partial H}{\partial p} = \frac{1}{a(x)}p = u'$$

which coincides with the system in Example (**??**).

1.3 The first integrals through the Hamiltonian

System (**??**) demonstrates that

$$\text{if } H = \text{ constant}(u_i), \quad \text{then } p_i = \text{ constant} \tag{19}$$

and

$$\text{if } H = \text{ constant}(p_i), \quad \text{then } u_i = \text{ constant} \tag{20}$$

This equations correspond to the fist integrals in the Euler equation

$$\frac{d}{dx}\frac{\partial L}{\partial u_i'} - \frac{\partial L}{\partial u_i} = 0, \quad i = 1, \ldots, N$$

If Lagrangian L is independent of u_i, $\frac{\partial L}{\partial u_i} = 0$, $\frac{\partial L}{\partial u_i'} =$ constant.

If Lagrangian is independent of u_i', $\frac{\partial L}{\partial u_i'} = 0$, then $\frac{\partial L}{\partial u_i} = 0$

Example 1.4 (Rotating mass 2) The Hamiltonian in the example **??** is

$$H = \frac{1}{2m}(p_\rho^2 + \frac{1}{\rho^2}p_\theta^2) + V(\rho) \tag{21}$$

The Hamiltonian is independent of θ, see (**??**); therefore p_θ is constant, $p_\theta = C_1$, and Hamiltonian becomes function of ρ and p_ρ only:

$$H = \frac{1}{2m}(p_\rho^2 + \frac{1}{\rho^2}C_1^2) + V(\rho) \tag{22}$$

Conservative system: Lagrangian is independent of x If $F = F(u, u')$, than

$$\hat{H}(u, p) = \text{ constant} \tag{23}$$

Indeed, compute the time derivative of the Hamiltonian using the chain rule

$$\frac{d}{dx}H(x, u, p) = \frac{\partial H}{\partial x} + \frac{\partial H}{\partial u}u' + \frac{\partial H}{\partial p}p' = \frac{\partial H}{\partial x}$$

because of equalities (**??**), $u' = \frac{\partial H}{\partial p}$ and $p' = -\frac{\partial H}{\partial u}$. If Lagrangian does not explicitly depend on x, the Hamiltonian is independent of x as well, $\frac{\partial H}{\partial x} = 0$ and we arrive at (**??**). This feature corresponds to the conservation of the total energy.

Example 1.5 (Rotating mass 3) The Hamiltonian (**??**) is independent of time t therefore is constant,

$$H = \frac{1}{2m}(p_\rho^2 + \frac{1}{\rho^2}C_1^2) + V(\rho) = C_2. \tag{24}$$

This equality allows to find p_ρ as a funtion of ρ:

$$p_\rho = \sqrt{2mC_2 - V(\rho) - \frac{1}{\rho^2}C_1^2}$$

Then using (**??**) we end up with the first-order equation for $\rho(t)$ that permit separation of variables

$$m\frac{d\rho}{dt} = \sqrt{2mC_2 - V(\rho) - \frac{1}{\rho^2}C_1^2}$$

Natural boundary conditions The natural or variational boundary conditions that are imposed at the endpoint b from the requirement of minimization of the functional, are $\frac{\partial L}{\partial u'} = 0$ at $x = b$. By definition of the impulse, it is rewritten as

$$p = 0 \quad \text{at } x = b;$$

Transversality condition The transversality condition (**??**) at the unknown endpoint $x = b$ of the trajectory $u(x)$ is expressed through Lagrangian $L(x, u, u')$ as

$$L - u' \frac{\partial L}{\partial u'} = 0$$

The expression in the left-hand side is Hamiltinian, therefore the condition takes a simple form:

$$H = 0 \quad \text{at } x = b.$$

The Hamiltonian for a conservative system is constant (**??**); therefore, there is no optimal endpoint for such systems.

Weierstrass-Erdmann condition This condition states that at all points of optimal trajectory, $\frac{\partial L}{\partial u'}$ is continuous. It translates into a statement that impulse p is continuous everywhere. Notice that by virtue of (**??**), p is differentiable.

Lagrangian and Hamiltonian Both functions describe the same process, but

- Hamiltonian is an algebraic function of differentiable arguments p and u, and Lagrangian is an expression for u, and it's derivative u', the derivative that may be discontinuous.

- Optimality conditions for Hamiltonian are expressed as a system of first-order differential equations in canonical form. Optimality conditions for Lagrangian are expressed as a system of second-order differential equations.

- Invariant properties and boundary conditions are more conveniently expressed through Hamiltonian.

- Lagrangian deals with the minimizer and its derivatives; its minimization is a realization of the minimal principle.

1.4 Hamiltonian for geometric optics

The results of study of geometric optics (Section **??**) can be conveniently presented using Hamiltonian. It is convenient to introduce the slowness $w(x, y) = \frac{1}{v(x,y)}$ - reciprocal to the speed v. Then the Lagrangian for the geometric optic problem is

$$L(x, y, y') = w\sqrt{1 + (y')^2} \quad y' > 0.$$

To find the canonical system, we use the outlined procedure: Define a variable p dual to $y(x)$ by the relation $p = \frac{\partial L}{\partial y'}$

$$p = \frac{wy'}{\sqrt{1 + (y')^2}}. \tag{25}$$

Solving for y', we obtain first canonical equation:

$$y' = \frac{p}{\sqrt{w^2 - p^2}} = \phi(x, y, p), \tag{26}$$

Excluding y' from expression for $L(x, y, y')$we find by means of (**??**), we find

$$L(x, y, y') = L_*(x, y, y'(p)) = \frac{w^2}{\sqrt{w^2 - p^2}}.$$

and recalling the representation for the solution y of the Euler equation

$$p' = \frac{\partial L}{\partial y} = \frac{\partial L_*}{\partial w}\frac{\partial w}{\partial y}$$

we obtain the second canonical equation:

$$p' = -\frac{w}{\sqrt{w^2 - p^2}}\frac{\partial w}{\partial y} \tag{27}$$

Hamiltonian Hamiltonian $H = p\phi - L_*(x, y, p)$ can be simplified to the form

$$H = -\sqrt{w^2 - p^2}$$

It satisfies the remarkably symmetric relation

$$H^2 + p^2 = w^2$$

that contains the whole information about the geometric optic problem. The elegancy of this relation should be compared with messy straightforward calculations that we previously did.

2 Hamiltonian and differential constraints

2.1 Differential constraints that introduce Hamiltonian

Here, we derive Hamiltonian with all its remarkable properties from the analysis of a constrained variational problem. The problem

$$I = \min_u \int_0^1 F(x, u, u')dx$$

for the vector-valued minimizer $u(x)$ can be presented as the constrained problem

$$I = \min_{u,v} \int_0^1 F(x, u, v)dx \quad \text{subject to } u' = v \tag{28}$$

where the constraint $u' = v$ specifies the differential dependence between two arguments of the Lagrangian. The last problem is naturally rewritten using Lagrange function $p = p(x)$:

$$I = \min_{u,v} \max_{p} J, \quad J = \int_0^1 \left[F(x,u,v) + p(u' - v) \right] dx \tag{29}$$

Integration by parts of the term $p\,u'$ in the integrand gives

$$J = \int_0^1 F_D(x,u,v,p)dx + p\,u|_0^1 \quad F_D(x,u,v,p) = \left[F(x,u,v) - p'u - p\,v \right]$$

Interchange the sequence of extremal operations in eqham2 and obtain the inequality:

$$I \geq \max_{p} I^D; \quad I^D = \min_{u,v} \int_0^1 F_D(x,u,v,p)dx + p\,u|_0^1 \tag{30}$$

Notice that the integrand for minimal problem I^D includes u and v but not their derivatives, therefore the minimization is performed independently in each point of the trajectory The stationarity conditions for I^D are are the coefficients by variations δu and δv are, respectively

$$\frac{\partial F}{\partial u} - p' = 0, \quad \frac{\partial F}{\partial v} - p = 0. \tag{31}$$

2.2 Transformation of stationarity conditions

Now, we can transform the problem in three different ways

Excluding Lagrange function p. Original Euler equation Exclude p and p' from (**??**). Differentiate second equation in (**??**) and substract the result from the first equation; obtain

$$\frac{d}{dx}\frac{\partial F}{\partial v} - \frac{\partial F}{\partial u} = 0, \quad u' = v$$

Thus, we return to the Euler equation in the original form.

Excluding the minimizer: Dual problem. Lower bound Exclude u and v from two equations (**??**) solving them for u and v: $u = \phi(p,p')$, $v = \psi(p,p')$.

Since $v = u'$, we we obtain the dual from of stationarity condition

$$\frac{d}{dx}\phi(p,p') - \psi(p,p') = 0$$

This is a second-order differential equation for p; the corresponding variational problem is

$$I \geq I^D; \quad I^D = \max_{p} \int_0^1 \left[F^D(x,p,p') \right] dx \tag{32}$$

where

$$F^D(p,p') = F(x,\phi,\psi) - p'\phi - p\psi \tag{33}$$

The dual problem (**??**) asks for maximum of the functional with Lagrangian $F^D(p,p')$, (**??**). Any trial function p that is consistent with the boundary conditions produces the lower bound of I.

Remark 2.1 (Lower bound) The duality is an essential tool because it provides the means to estimate the lower bound of the variational problem. The upper bound is easy to obtain: every trial function u_{trial} consistent with the main boundary conditions provides such a bound to a minimal variational problem. To find the lower bound, we use the dual problem (**??**). This relation implies that any trial function p_{trial} with the main boundary conditions corresponds to the lower bound of the functional.

$$\int_a^b F^D(x,u,p_{trial})dx \le I \le \int_a^b F(x,u_{trial},p)dx \quad \forall p_{trial}, u_{trial} \tag{34}$$

The difference between the upper and lower bound provide the measure of the preciseness of both approximations:

Excluding derivatives: Hamiltonian. canonical system Excluding v from (**??**): $v=\rho(u,p)$ we express the problem through the Hamiltonian $H(u,p)$

$$I^H = \min_u \max_p \int_0^1 \left[u'p - H(u,p)\right] dx \tag{35}$$

where

$$H(u,p) = \rho(u,p)p - F(x,u,\rho(u,p)) \tag{36}$$

Necessary conditions for maximum in (**??**) with respect to p recover the condition (**??**):$u' = \frac{\partial H}{\partial p}$. To recover the second condition, $p' = \frac{\partial H}{\partial u}$, we integrate by parts the term $u'p$ in the integrand in (**??**). This argument explains the remarkable feature of Hamiltonian as the potential to the canonical system.

2.3 Constraints in the form of differential equations

$$\min_u \int_a^b F(u)dx + \Psi(u(b)) \quad \text{subject to} \tag{37}$$

$$u_i' = f_i(x,u), \quad i=1,\dots,n, \quad u(a) = U_a \tag{38}$$

where $u(x)$ is vector of minimizers.

The Lagrangian has the form

$$L = F(u) + p^T(u' - f(x,u)$$

Hamiltonian is computed as

$$H = p^T u' - L = -F(u) + p^T f(x,u) \tag{39}$$

One chan check that

$$\frac{\partial H}{\partial p} = f(x, u) = u'$$

Equations for p (adjoint system) are linear with respect to p::

$$p_i' = -\frac{\partial H}{\partial u} = p^T \frac{\partial f}{\partial u_i} - \frac{\partial F}{\partial u}$$

Compementary boundary conditions at the endpoint $x = b$ are:

$$p + \frac{\partial \Psi}{\partial u} = 0, \quad x = b.$$