# Variational Principles IB Easter

# 1 Multi-variable function

- Stationary point $\implies \nabla f = \mathbf{0}$
- Max, min, saddle: check eigenvalues of Hessian matrix

# 2 Convexity, Extremising functions $\mathbb{R}^n \to \mathbb{R}$

- Convex set; convex, strictly convex, concave function etc.
- (Chord connecting two points of convex set lies entirely in the set, chord of graph of convex function lies above graph of function)
- Stationary point of convex function is global minimum (may not be unique point)

### Alternative characterisation of convexity

- Once differentiable function:
  $f$ is convex
  $$\iff f(y) \geq f(x) + (y-x) \cdot \nabla f(x)$$
  (graph lies above tangent plane)
  $$\iff (y-x) \cdot (\nabla f(y) - \nabla f(x)) \geq 0$$
  (in case $n = 1$, condition means $f'$ monotonic increasing)
- Twice differentiable: convex iff Hessian matrix non-negative definite
  (no equivalence for strictly convex, $H$ positive definite $\implies$ strict convexity but no reverse implication)
- Extremising function under constraints:
  Extremise $f(\mathbf{x})$ while fixing $g(\mathbf{x}) = L$:
  By Lagrange multiplier, extremise $h(\mathbf{x}, \lambda) = f(\mathbf{x}) - \lambda(L - g(\mathbf{x}))$

# 3 Legendre Transform

Given function $f : \mathbb{R}^n \to \mathbb{R}$, the Legendre Transform of $f$ is

$$f^*(\mathbf{p}) = \sup_{\mathbf{x}} (\mathbf{p} \cdot \mathbf{x} - f(\mathbf{x})),$$

over the domain $D \subseteq \mathbb{R}^n$ on which the sup is finite.

- $f^*$ is always convex
- If $f$ is convex and differentiable, then $f(\mathbf{x}) - \mathbf{p} \cdot \mathbf{x}$ is convex.
  So any stationary point of $\mathbf{p} \cdot \mathbf{x} - f(\mathbf{x})$ is global max (unique if $f$ is strictly convex), which occurs at $\mathbf{x}(\mathbf{p})$ that satisfies

  $$\nabla f(\mathbf{x}) = \mathbf{p}$$

  In this case $f^*(p) = \mathbf{p} \cdot \mathbf{x}(\mathbf{p}) - f(\mathbf{x}(\mathbf{p}))$
- $f^{**} = f$ if $f$ is convex

## Application to Thermodynamics

$$\mathrm{d}U = T\mathrm{d}S - P\mathrm{d}V$$

Legendre transform changes independent variables:
$U(S, V)$ becomes $F(T, V)$, and $H(S, P)$

- Helmholtz Free Energy:

  $$F(T, V) = \min_S (U(S, V) - TS) = -U^*(S, V)$$

  Legendre transform of $U$ with respect to $S$, fixing $V$
  The independent variable $T$ is temperature since the min is attained when $T = \frac{\partial U}{\partial S}\Big|_V$
  Get

  $$\mathrm{d}F = -S\mathrm{d}T - P\mathrm{d}V$$
- Enthalpy:

  $$H(S, P) = \min_V (U(S, V) + PV) = -U^*(-P, S),$$

  Legendre transform of $U$ with respect to $V$, with $S$ fixed
  The independent variable $P$ is indeed pressure since min attained when $P = -\frac{\partial U}{\partial V}\Big|_S$

  Get

  $$\mathrm{d}H = T\mathrm{d}S + V\mathrm{d}P$$

- Gibbs Free Energy:

$$G(T,P) = H(S,P) - TS,$$

where $S$ satisfies $T = \frac{\partial H}{\partial S}\big|_P$ , Legendre transform w.r.t. $S$

# 4 Extremising functional

- Finding "stationary" points of functional (max, min, saddle):

$$L[y] = \int_\alpha^\beta f(x,y,y')dx$$

subject to boundary condition that cause boundary term to vanish

- Taylor expand to first order, integrate by parts:

$$L[y+\varepsilon\eta] - L[y] = \varepsilon \int_\alpha^\beta \eta \left( \frac{\partial f}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial f}{\partial y'} \right) \mathrm{d}x + O(\varepsilon^2)$$

- Functional derivative/Euler-Lagrange equation:

$$\frac{\delta L[y]}{\delta y} = \frac{\partial f}{\partial y} - \frac{\mathrm{d}}{\mathrm{d}x}\frac{\partial f}{\partial y'} = 0$$

- First integrals if $f$ does not depend explicitly on $y$, or $x$

## Multiple dependent variables

Extremise

$$L[\mathbf{y}] = \int_\alpha^\beta f(x, y_1, \ldots, y_n, y_1', \ldots, y_n')\,\mathrm{d}x,$$

with appropriate boundary conditions

- Generalisation: Use Euler-Lagrange on each dependent variable
- Modification for first integrals:
  - $f$ no explicit dependence on some $y_i$: get first integral $\frac{\partial f}{\partial y_i'} =$ constant
  - $f$ no explicit dependence on $x$: get first integral $f - \sum y_i' \frac{\partial f}{\partial y_i'} =$ constant

## Multiple independent variables

Find function $\mathbf{\Phi} : D \subseteq \mathbb{R}^m \to \mathbb{R}^n$ fixed at boundary that extremises

$$F[\mathbf{\Phi}] = \int \cdots \int_D f(x_1, \ldots x_m, \mathbf{\Phi}, \nabla \mathbf{\Phi}) \, \mathrm{d}x_1 \ldots \mathrm{d}x_m,$$

where $\nabla \mathbf{\Phi} = \left( \frac{\partial \mathbf{\Phi}_i}{\partial x_j} \right)_{ij}$

- Taylor expand $f$, write integrand as a divergence $+ \, \eta \cdot (\frac{\delta F}{\delta \Phi})$
- Integral of divergence vanishes
- Euler-Lagrange give PDEs

## Euler-Lagrange for higher derivatives

For example: Extremise

$$F[x] = \int_\alpha^\beta f(t, \dot{x}, \ddot{x}) \, \mathrm{d}t,$$

with $x, \dot{x}$ fixed at boundary

Taylor Expand integrand, integration by parts: get

$$\delta F[x] = \int_\alpha^\beta \delta x \underbrace{\left( \frac{\partial f}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}x} \frac{\partial f}{\partial \dot{x}} + \frac{\mathrm{d}^2}{\mathrm{d}x^2} \frac{\partial f}{\partial \ddot{x}} \right)}_{\frac{\delta F}{\delta x}} \mathrm{d}t$$

## Extremising with constraints

Extremise

$$F[y] = \int_\alpha^\beta f(x, y, y') \, \mathrm{d}x$$

under functional constraint

$$G[y] = \int_\alpha^\beta g(x, y, y') \, \mathrm{d}x = K$$

- Use Lagrange multiplier: Extremise

$$L[y] = \int_\alpha^\beta f(x, y, y') - \lambda g(x, y, y') \, \mathrm{d}x = F[y] - \lambda G[y]$$

Extremise

$$F[\mathbf{x}] = \int_{\alpha}^{\beta} f(t, \mathbf{x}, \mathbf{x}')\, \mathrm{d}t$$

under function constraint $g(\mathbf{x}) = 0$ for all $t$

- Need Lagrange multiplier $\lambda(t)$ that changes with $t$:

$$\Phi[\mathbf{x}, \lambda] = \int_{\alpha}^{\beta} \left(f(t, \mathbf{x}, \mathbf{x}') - \lambda(t) g(\mathbf{x})\right)\, \mathrm{d}t$$

# 5 Example, variational principles

- Geodesic (minimise distance): Euclidean plane (straight line), sphere (great circle), general surface
- Minimal surface (minimise surface area): e.g. catenoid of soap film
- Brachistochrone: shortest travel time (cycloid)
- Fermat's Principle: least time $\implies$ Snell's Law
- Minimise potential energy (e.g. catenary)
- Dido problem (isoperimetric problem, maximise area)
- Sturm-Liouville problem
- Lagrangian (Old) principle of least action: Minimises $m \int v\, \mathrm{d}l$
- Hamilton's principle: action $= \int L\, \mathrm{d}t$

**Sturm-Liouville Problem**

Given $\rho(x), w(x) \geq 0$, extremise

$$F[y] = \int_{\alpha}^{\beta} \rho(x)(y')^2 + \sigma(x) y^2 \mathrm{d}x,$$

subject to

$$G[y] = \int_{\alpha}^{\beta} w(x) y^2 \mathrm{d}x = 1$$

and fixed boundary of $y$

- Use Lagrange multiplier, Euler Lagrange gives

$$-\frac{\mathrm{d}}{\mathrm{d}x}(\rho(x)y') + \sigma(x)y = \lambda w(x)y$$

- Extremal are eigenfunctions of Sturm-Liouville operator

$$\mathcal{L} = -\frac{\mathrm{d}}{\mathrm{d}x}\left(\rho(x)\frac{\mathrm{d}}{\mathrm{d}x}\right) + \sigma(x),$$

extremal $y$ satisfy

$$\mathcal{L}y = 2wy$$

- If also $\sigma(x) > 0$, then $F[y] \geq 0$, so minimum of $F[y]/G[y]$ is smallest eigenvalue of $\mathcal{L}$ (Check notes again for boundary term)

# 6 Formulation of Mechanics

## Lagrangian Mechanics

- Lagrangian $L = T - V$ in generalised coordinates
- Hamilton's Principle: Trajectory is stationary point of action (not actually minimiser) with fixed endpoints

$$A[\mathbf{x}] = \int_{t_1}^{t_2} L \,\mathrm{d}t$$

- Lagrange's Equation

$$\frac{\partial L}{\partial x_i} = \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{x}_i}\right)$$

- Implies Newton's 2nd Law
- If potential energy $V$ is independent of time, get conservation of energy

## Noether's Theorem

(More details in Townsend's notes p.35)
If $\mathbf{y} = (y_1, \dots y_n)$ extremises functional $F[\mathbf{y}] = \int_\alpha^\beta f(x, \mathbf{y}, \dot{\mathbf{y}}) \,\mathrm{d}x$, and there is 1-parameter continuous symmetry $y_i(x) \mapsto Y_i(s, x)$ such that

$$\frac{\mathrm{d}}{\mathrm{d}s} f(x, \mathbf{Y}(s,x), \dot{\mathbf{Y}}(s,x)) = 0, \text{ and } Y_i(0,x) = y_i(x)$$

Get first integral:

$$\sum_{i=1}^{n} \frac{\partial f}{\partial y_i'} \frac{\partial Y_i}{\partial s}\bigg|_{s=0} = \text{constant}$$

(Invariance under e.g. translation, rotation give conservation laws)

## Hamiltonian Mechanics

Hamiltonian = Legendre transform of Lagrangian $L(\mathbf{q}, \dot{\mathbf{q}}, t)$ with respect to velocity $\dot{\mathbf{q}}$ (in generalised coordinates):

$$\begin{aligned} H(\mathbf{q}, \mathbf{p}, t) &= \sup_{\dot{\mathbf{q}}} [\mathbf{p} \cdot \dot{\mathbf{q}} - L(\mathbf{q}, \dot{\mathbf{q}}, t)] \\ &= \mathbf{p} \cdot \dot{\mathbf{q}}(\mathbf{p}) - L(\mathbf{q}, \dot{\mathbf{q}}(\mathbf{p}), t), \text{ where } \dot{\mathbf{q}}(\mathbf{p}) \text{ satisfies} \end{aligned}$$

$$\mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{q}}}, \text{ i.e. } p_i = \frac{\partial L}{\partial \dot{q}_i}$$

- New independent variable $\mathbf{p}$ is generalised momentum
- In one particle scenario, Hamiltonian is total energy $(T + V)$
- Hamilton's equations:

$$\begin{aligned} \mathrm{d}H &= \frac{\partial H}{\partial q_i} \mathrm{d}q_i + \frac{\partial H}{\partial p_i} \mathrm{d}p_i + \frac{\partial H}{\partial t} \mathrm{d}t \\ &= \frac{\partial L}{\partial q_i} \mathrm{d}q_i + \left[\dot{q}_i + \left(p_j - \frac{\partial L}{\partial \dot{q}_j}\right) \frac{\partial \dot{q}_j}{\partial p_i}\right] \mathrm{d}p_i - \frac{\partial L}{\partial t} \mathrm{d}t \\ &= (\dot{p}_i)\, \mathrm{d}q_i + (\dot{q}_i)\, \mathrm{d}p_i - \frac{\partial L}{\partial t} \mathrm{d}t. \end{aligned}$$

  where $p_j = \frac{\partial L}{\partial \dot{q}_j}$ by above, and $\frac{\partial L}{\partial q_i} = \frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial L}{\partial \dot{q}_i} = \dot{p}_i$ by Lagrange's equation

  Matching terms give

$$\frac{\partial H}{\partial \mathbf{q}} = -\dot{\mathbf{p}}, \qquad \frac{\partial H}{\partial \mathbf{p}} = \dot{\mathbf{q}}, \qquad \frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t}$$

  (Be careful of which variables held fixed in partial differentiation)

- Hamilton's equations can also be obtained from E-L equations of a variational principle, extremising

$$S[\mathbf{q}, \mathbf{p}] = \int \{\mathbf{p} \cdot \mathbf{q} - H(\mathbf{q}, \mathbf{p}, t)\}\ \mathrm{d}t$$

# 7 Second variation

To extremise $F[y] = \int_\alpha^\beta f(x, y, y')\,\mathrm{d}x$, with fixed ends.

- Taylor expand $F[y+\varepsilon\eta] - F[y]$ to second order, about stationary point $y$:

$$F[y+\varepsilon\eta]-F[y] = \varepsilon^2 \underbrace{\frac{1}{2}\int_\alpha^\beta \left(\eta^2 \frac{\partial^2 f}{\partial y^2} + (\eta')^2 \frac{\partial^2 f}{\partial y'^2} + 2\eta\eta' \frac{\partial^2 f}{\partial y\,\partial y'}\right)\mathrm{d}x}_{\delta^2 F[y,\eta]} + O(\varepsilon^3)$$

- Using by parts on mixed term:

$$\delta^2 F[y,\eta] = \frac{1}{2}\int_\alpha^\beta \left\{ \underbrace{\left(\frac{\partial^2 f}{\partial y^2} - \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial^2 f}{\partial y\,\partial y'}\right)\right)}_{Q}\eta^2 + \underbrace{\frac{\partial^2 f}{\partial y'^2}}_{P}(\eta')^2 \right\}\mathrm{d}x$$

- If $y$ satisfies E-L, and $\delta^2 F[y,\eta] \geq 0$ for any $\eta$ that vanishes at endpoints, then $y$ is a local minimiser of $F[y]$

## Conditions for local minimum

- Legendre condition: $y$ is a local minimum $\implies P = \frac{\partial^2 f}{\partial y'^2} \geq 0$; otherwise, can find $\eta$ with small magnitude but large $(\eta')^2$ to give contradiction

  (necessary, not sufficient)

- $P > 0$ and $Q \geq 0$ sufficient for local minimum

- Rewrite

$$Q\eta^2 + P(\eta')^2 = Q\eta^2 + (P\eta\eta')' - \eta(P\eta')'$$

  In terms of Sturm-Liouville operator

$$\delta^2 F[y,\eta] = \frac{1}{2}\int_\alpha^\beta \eta\,\underbrace{(-(P\eta')' + Q\eta)}_{\mathcal{L}(\eta)}\,\mathrm{d}x$$

  If $\mathcal{L}$ has a negative eigenvalue, with eigenfunction $\eta$ that vanishes at endpoints, i.e.

$$\mathcal{L}(\eta) = -\omega^2\eta, \quad \eta(\alpha) = \eta(\beta) = 0,$$

  then $y$ is not a local minimiser

**Jacobi condition**

It is known that $P > 0$ is not sufficient for local minimum, but when does it fail?

- For any differentiable $\phi$, have

$$0 = \int_\alpha^\beta (\phi\eta^2)' \,\mathrm{d}x = \int_\alpha^\beta [2\phi\eta\eta' + \phi'\eta^2] \,\mathrm{d}x,$$

- Add it to $\delta^2 F[y, \eta]$, complete the square (assuming $P > 0$):

$$\delta^2 F[y, \eta] = \frac{1}{2} \int_\alpha^\beta \left[ P \left( \eta' + \frac{\phi\eta}{P} \right)^2 + \left( Q + \phi' - \frac{\phi^2}{P} \right) \eta^2 \right] \mathrm{d}x$$

- If can choose $\phi$ to make the second term vanish, then $\delta^2 F[y, \eta] > 0$. This sufficient condition is given by a Ricatti equation

$$\phi^2 = P(Q + \phi')$$

- Transform the equation, by letting $\phi = -P\frac{u'}{u}$, get Jacobi accessory equation

$$-(Pu')' + Qu = 0$$

  Need to find solution $u$ to this Strum-Liouville equation s.t. $u(x) \neq 0$ for $\alpha < x < \beta$, which might not exist for interval too large