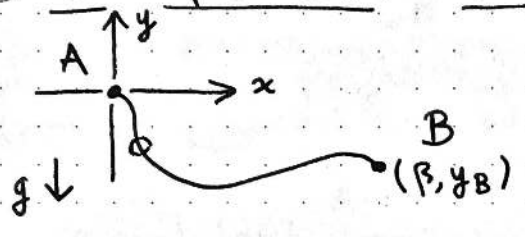


# Variational Principles

## § 0. Motivation

### ● Example 0.1 The Brachistochrone



A particle starts at rest and slides along the wire from A to B under the influence of gravity.

Find the shape of the wire st the travel time is minimal.

1696 Johan Bernoulli

$T+V = \text{const.}$   $\frac{mv^2}{2} + mgy = 0$  by computing at A

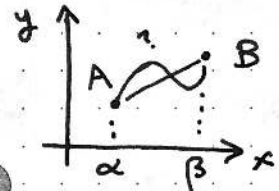
● Time =  $\int_A^B dt = \int_0^\beta \frac{dl}{v(x,y)} = \int_0^\beta \frac{\sqrt{1+(y')^2}}{v}$

Now,  $v = \sqrt{-2gy}$ , to give

Time =  $\int_0^\beta \frac{\sqrt{1+(y')^2}}{\sqrt{-2gy}} dx$

### Example 0.2 Geodesic = shortest path (if it exists)

between two points on a surface  $\Sigma \subset \mathbb{R}^3$ . Take  $\Sigma = \mathbb{R}^2$



$D = \int_\alpha^\beta \sqrt{1+(y')^2} dx$

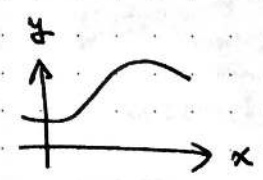
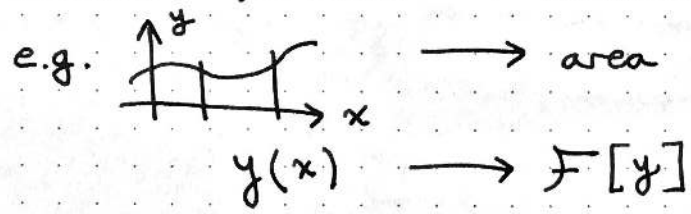
minimise D with  $y(\alpha) = y_A, y(\beta) = y_B$

● Maths In both cases we aim to minimise

$F[y] = \int_\alpha^\beta f(x, y, y') dx$  (0.1)

(0.1) is an example of a functional function: number  $\rightarrow$  number

functional: function  $\rightarrow$  number



Books  
Gelfand & Fomin "Calculus of Variations"  
DAMTP notes (Townsend)  
This course (diff order 5)

L1.2

Calculus of variations finding critical points of functionals

(a part of functional analysis)

Need to specify a class of functions  $y(x)$  for which (0.1) is to be minimised.

e.g.  $C(\mathbb{R})$  = space of continuous functions on  $\mathbb{R}$

$C^k(\mathbb{R})$  = " continuously  $k$ -times diff'ble

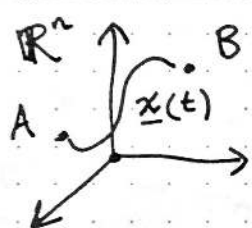
$C^k_{(\alpha, \beta)}(\mathbb{R})$  = " supported on  $(\alpha, \beta)$

Variational principles (?) = principles of nature where the laws reduce to minimising (maximising) a functional

Example 0.3 Fermat's principle "Light travels between

A and B along a path which minimises travel time"

Example 0.4 Principle of least action


$\mathbb{R}^n$    $T = \text{kinetic energy (e.g. } \frac{m|\dot{x}|^2}{2} \text{)}$

$V = \text{potential energy (e.g. } V(x) \text{)}$

$$\text{Action } S[x] = \int_{t_1}^{t_2} (T - V) dt$$

Then action is stationary along the paths taken by the particle.  $\Rightarrow \ddot{x} = -\nabla V$

Leibniz on Example 0.3 "We live in the best of all worlds"

Theology alert! 

Feynman on Example 0.3 "This is wrong in Quantum Theory"

A particle takes all possible paths with different probabilities.

This course

- 1) Find necessary conditions for  $y(x)$  to minimise  $F[y]$   
 $\rightarrow$  Euler-Lagrange equations
- 2) Lots of examples (geometry, physics)  
Problems with constraints (e.g. find area maximising shape)
- 3) Some sufficient conditions for min/max (2<sup>nd</sup> variation)

L2.1

§ 1 Calculus on  $\mathbb{R}^n$ 

- $f \in C^2(\mathbb{R}^n)$ ,  $f: \mathbb{R}^n \rightarrow \mathbb{R}$ , continuous <sup>2nd</sup> partial derivatives
- $\underline{a} \in \mathbb{R}^n$  critical point i.e.  $\nabla f|_{\underline{a}} \equiv (\partial_1 f, \dots, \partial_n f)|_{\underline{a}} = \underline{0}$
- where  $\partial_i = \partial/\partial x_i$  for  $i = 1, \dots, n$

Expand around  $\underline{a}$ :  $f(\underline{x}) = f(\underline{a}) + (\underline{x} - \underline{a}) \cdot \nabla f|_{\underline{a}} + \frac{1}{2} \sum_{i,j} (x^i - a^i)(x^j - a^j) \frac{\partial^2 f}{\partial x^i \partial x^j} |_{\underline{a}} + O(|\underline{x} - \underline{a}|^3)$

Hessian matrix  $H$ ,  $H_{ij} \equiv \frac{\partial^2 f}{\partial x^i \partial x^j} = H_{ji}$  since  $C^2$

- Shift the origin to  $\underline{a} = \underline{0}$ . Diagonalise  $H(\underline{0})$  via an orthogonal transformation  $R$ :

$$H'(\underline{0}) = R^T H(\underline{0}) R = \begin{pmatrix} \lambda_1 & & 0 \\ & \lambda_2 & \\ 0 & & \ddots \\ & & & \lambda_n \end{pmatrix}$$

Go back to Taylor expansion:

$$f(\underline{x}) - f(\underline{0}) = \frac{1}{2} \sum \lambda_i (x^i)^2 + O(|\underline{x}|^3)$$

- i) If all  $\lambda_i > 0$ , then  $f(\underline{x}) - f(\underline{0}) > 0 \forall \underline{x} \neq \underline{0}$  (to 2<sup>nd</sup> order)
- $\underline{x} = \underline{0}$  is a local minimum
- ii) If all  $\lambda_i < 0$  have a local maximum
- iii) Some  $\lambda_i > 0$ , some  $\lambda_i < 0$  give saddle point
- iv) Some  $\lambda_i = 0$ , look at higher order terms in series
- Special case  $n=2$ .  $\det(H) = \lambda_1 \lambda_2$ ,  $\text{Tr}(H) = \lambda_1 + \lambda_2$
- (i)  $\det H > 0$ ,  $\text{Tr} H > 0$  local minimum
- (ii)  $\det H > 0$ ,  $\text{Tr} H < 0$  local maximum
- (iii)  $\det H < 0$  saddle point
- (iv)  $\det H = 0$  look at higher order terms

Remark: If  $f: D \rightarrow \mathbb{R}$  with  $D \subseteq \mathbb{R}^n$  then need to examine the boundary of  $D$  for global max/min

Examples 1.1) Harmonic functions on  $D \subseteq \mathbb{R}^2$

$$\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} = 0 \Rightarrow \det H < 0 \text{ so min/max on } \partial D$$

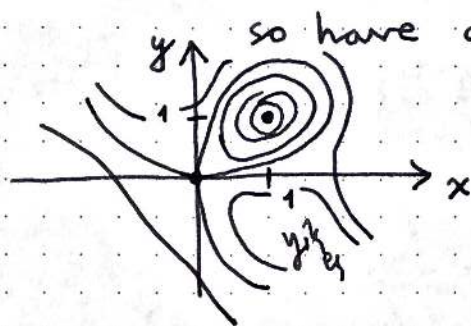
1.2)  $f(x, y) = x^3 + y^3 - 3xy$

$\nabla f = (3(x^2 - y), 3(y^2 - x))$  so get  $(0, 0)$  and  $(1, 1)$

$H = \begin{pmatrix} 6x & -3 \\ -3 & 6y \end{pmatrix}$   $H|_{(0,0)}$  has det  $-9$ , so saddle  
 $H|_{(1,1)}$  has det  $27$ , trace  $12$

so have a minimum point

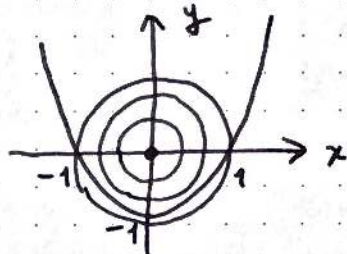
Contour plot



near  $(0, 0)$   
 $f \sim -3xy$

### § 1.1 Constraints and Lagrange Multipliers

Example Find a circle in  $\mathbb{R}^2$ , centred at the origin which has minimal radius and intersects the parabola  $y = x^2 - 1$



Two approaches

(1) Solve the constraint:  $y = x^2 - 1$

$$f(x, y) = x^2 + y^2 = x^2 + (x^2 - 1)^2 \\ = x^4 - x^2 + 1 = \hat{f}(x)$$

$$\frac{d\hat{f}}{dx} = 4x^3 - 2x = 2x(2x^2 - 1) \text{ is zero at } x = 0, \pm \sqrt{2}/2$$

$$f = 1 \quad f = \frac{3}{4} \quad \cup$$

(2) Lagrange multipliers

Define  $h(x, y, \lambda) = f(x, y) - \lambda g(x, y)$  where  $\lambda$  is the Lagrange multiplier, and  $g(x, y) = 0$  is the constraint.

Extremise  $h$  wrt  $x, y, \lambda$  without constraints

$$h = x^2 + y^2 - \lambda(y - x^2 + 1)$$

$$\frac{\partial h}{\partial x} = 2x + 2x\lambda$$

$$\frac{\partial h}{\partial y} = 2y - \lambda$$

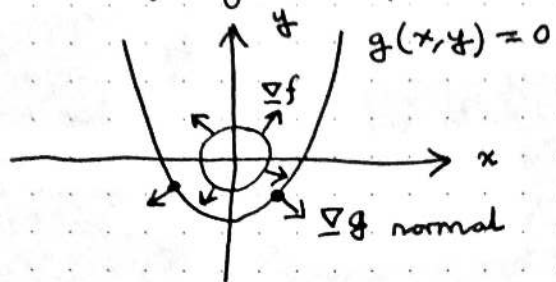
$$\frac{\partial h}{\partial \lambda} = x^2 - y - 1$$

L2.3

$$2x(1+2y) = 0 \quad \text{so } x=0 \text{ or } y = -\frac{1}{2}$$

Then in third equation,  $x=0 \Rightarrow y=-1$  and  $y=-\frac{1}{2} \Rightarrow x = \pm \frac{1}{\sqrt{2}}$

Why do Lagrange multipliers work? Geometry



Then at critical points,

$\nabla f$  and  $\nabla g$  are parallel

So  $\nabla f = \lambda \nabla g$  and

$$\nabla(f - \lambda g) = 0. \quad \circ$$

$\nabla h = 0$  follows through

In general  $f: \mathbb{R}^n \rightarrow \mathbb{R}$ , subject to  $K$  constraints  $g_\alpha(x) = 0$

where  $g_\alpha: \mathbb{R}^n \rightarrow \mathbb{R}$ ,  $\alpha = 1, \dots, K$

$$\text{Define } h(x_1, \dots, x_n, \underbrace{\lambda_1, \dots, \lambda_K}_{K \text{ Lagrange } \text{bois}}) = f - \sum_{\alpha=1}^K \lambda_\alpha g_\alpha$$

Extremise  $h$ :  $\frac{\partial h}{\partial x_i} = 0$  and  $\frac{\partial h}{\partial \lambda_\alpha} = 0$   $n+K$  eqns

Eliminate  $\lambda_\alpha$  and solve for critical points

## § 2 The Euler-Lagrange Equations

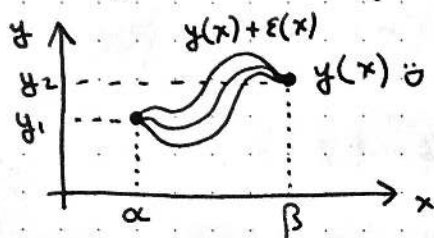
Find extrema of the functional  $(0, 1): y: \mathbb{R} \rightarrow \mathbb{R}$

$$F[y] = \int_{\alpha}^{\beta} f(x, y, y') dx \quad (2.1)$$

$$y \in C_{[\alpha, \beta]}^2(\mathbb{R})$$

↑  
just "on"  $[\alpha, \beta]$

subject to  $y(\alpha) = y_1, y(\beta) = y_2$



Lemma Let  $g: [\alpha, \beta] \rightarrow \mathbb{R}$  be continuous, and such that

$$\int_{\alpha}^{\beta} g(x) \eta(x) dx = 0 \quad \text{for all continuous } \eta: [\alpha, \beta] \rightarrow \mathbb{R}$$

such that  $\eta(\alpha) = \eta(\beta) = 0$ .

Then  $g(x) \equiv 0$  on  $[\alpha, \beta]$ .

Proof Assume  $\exists \bar{x} \in [\alpha, \beta]$  such that  $g(\bar{x}) \neq 0$  (say  $g(\bar{x}) > 0$ )

Then  $\exists c > 0, [x_1, x_2] \subset [\alpha, \beta]$  such that  $\bar{x} \in [x_1, x_2]$  and  $g(x) > c$  on  $[x_1, x_2]$ .

$$\text{Define } \eta(x) = \begin{cases} (x-x_1)(x_2-x) & \text{if } x \in [x_1, x_2] \\ 0 & \text{if } x \notin [x_1, x_2] \end{cases} \quad (2.2)$$

$$\text{Then } \int_{\alpha}^{\beta} g(x) \eta(x) dx > \int_{x_1}^{x_2} c (x-x_1)(x_2-x) dx > 0. \quad \#$$

So no such  $\bar{x}$  exists, and  $g \equiv 0$ . □

Assume that (2.1) admits an extremum, and replace  $y$  by  $y(x) + \varepsilon \eta(x)$  in (2.1), where  $\eta(\alpha) = \eta(\beta) = 0$ .

$$F[y + \varepsilon \eta] = \int_{\alpha}^{\beta} f(x, y + \varepsilon \eta, y' + \varepsilon \eta') dx$$

$$= F[y] + \varepsilon \int_{\alpha}^{\beta} \left( \frac{\partial f}{\partial y} \eta + \frac{\partial f}{\partial y'} \eta' \right) dx + O(\varepsilon^2)$$

↳ def<sup>n</sup>?  
of  
derivative

For an extremum, the linear term in  $\varepsilon$  should vanish,

$$\text{i.e. } \left. \frac{dF}{d\varepsilon} \right|_{\varepsilon=0} = 0$$

L3.2

So  $0 = \int_{\alpha}^{\beta} \left( \frac{\partial f}{\partial y} \eta + \frac{\partial f}{\partial y'} \eta' \right) dx$ . Integrate second term.

$$0 = \int_{\alpha}^{\beta} \left( \frac{\partial f}{\partial y} \eta - \frac{d}{dx} \left( \frac{\partial f}{\partial y'} \right) \eta \right) dx + \underbrace{\left[ \eta \frac{\partial f}{\partial y'} \right]_{\alpha}^{\beta}}_{\text{zero as } \eta \text{ vanishes on } \alpha, \beta}$$

zero  $\forall \eta$

By Lemma, with  $g = \frac{\partial f}{\partial y} - \frac{d}{dx} \left( \frac{\partial f}{\partial y'} \right)$ , obtain

Theorem If an extremum  $y \in C^2(\mathbb{R})$  of (2.1) exists, then it satisfies

$$\boxed{\frac{d}{dx} \left( \frac{\partial f}{\partial y'} \right) - \frac{\partial f}{\partial y} = 0} \quad (2.3)$$

Remarks 1) (2.3) is a 2<sup>nd</sup> order ODE for  $y(x)$ , subject to boundary conditions  $y(\alpha) = y_1, y(\beta) = y_2$

It is called the Euler-Lagrange equation ( $\square$ : Lagrange Euler 1745)

2)  $\eta$  in (2.2) is an example of a "bump" function which was continuous. A  $C^k(\mathbb{R})$  bump function could be

$$\eta(x) = \begin{cases} [(x-x_1)(x-x_2)]^{k+1} & \text{if } x \in [x_1, x_2] \\ 0 & \text{otherwise} \end{cases}$$

3) Notation and terminology. LHS of (2.3) is called the functional derivative and denoted by  $\frac{\delta F[y]}{\delta y(x)}$ . Some books/notes (e.g. P Townsend)

replace  $\varepsilon \eta(x) \rightarrow \delta y(x)$ . "a small variation"

$$F[y + \delta y] = F[y] + \delta F[y] \quad \text{where} \quad \delta F[y] = \int_{\alpha}^{\beta} \frac{\delta F[y]}{\delta y(x)} \delta y(x) dx$$

4) Be careful with derivatives.

$$\text{In (2.3)} \quad \frac{\partial}{\partial x} \Big|_{x, y'} \quad \frac{\partial}{\partial y} \Big|_{x, y'} \quad \frac{\partial}{\partial y'} \Big|_{x, y}$$

Take  $h(x, y, y')$ . Then

$$\frac{dh}{dx} = \frac{\partial h}{\partial x} + \frac{\partial h}{\partial y} \frac{dy}{dx} + \frac{\partial h}{\partial y'} \frac{dy'}{dx}$$

L3.3

So  $\frac{d}{dx} = \frac{\partial}{\partial x} + y' \frac{\partial}{\partial y} + y'' \frac{\partial}{\partial y'}$ , the total derivative.

For example, take  $h(x, y, y') = x((y')^2 - y^2)$ .

Then  $\frac{\partial h}{\partial x} = (y')^2 - y^2$      $\frac{\partial h}{\partial y} = -2xy$      $\frac{\partial h}{\partial y'} = 2xy'$ , and

$$\frac{dh}{dx} = (y')^2 - y^2 - 2y'xy + 2y''xy' \quad \ddot{\circ}$$

### § 2.1 The first integrals of E-L (Euler-Lagrange)

In some cases, it is possible to reduce (2.3) to a 1<sup>st</sup> order

ODE. (i) Assume  $\frac{\partial f}{\partial y} = 0$ , i.e.  $f = f(x, y')$

Then (2.3) implies  $\frac{d}{dx} \left( \frac{\partial f}{\partial y'} \right) = 0$ ,

so  $\frac{\partial f}{\partial y'} = \text{const.}$  (a first integral of 2.3) (2.4)

Example 2.1 geodesics on  $\mathbb{R}^2$

$$F[y] = \int_{\alpha}^{\beta} \underbrace{(1 + (y')^2)^{\frac{1}{2}}}_{f(y')} dx$$



So have, by (2.4),  $\frac{\partial f}{\partial y'} = \frac{y'}{\sqrt{1+y'^2}} = \text{const}$

So  $y' = m$  (const.)

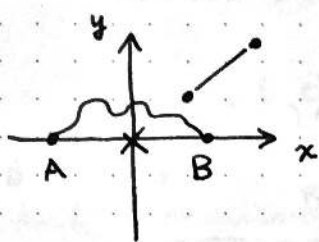
And  $y$  is a straight line  $\ddot{\circ}$



L4.1

Recall the Euler-Lagrange equation  $\frac{d}{dx} \left( \frac{\partial f}{\partial y'} \right) = \frac{\partial f}{\partial y}$  (2.3)

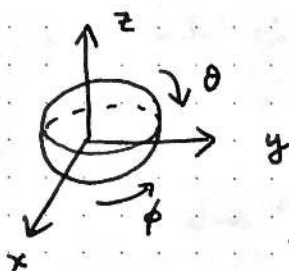
● Geodesics on  $\mathbb{R}^2 =$  straight lines  $y = mx + c$



Consider  $\mathbb{R}^2 \setminus \{0\}$

Then no geodesic  $A \rightarrow B$

Example Geodesics on a sphere  $S^2 \subset \mathbb{R}^3$ ,  $x^2 + y^2 + z^2 = 1$



Parametrise via  $\theta$  and  $\phi$  so

$$x = \sin \theta \cos \phi, \quad y = \sin \theta \sin \phi, \quad z = \cos \theta$$

$$ds^2 = dx^2 + dy^2 + dz^2 = d\theta^2 + \sin^2(\theta) d\phi^2$$

Treat  $\phi$  as a function of  $\theta$  to get

$$F[\phi] = \int_{\theta_1}^{\theta_2} \sqrt{1 + \sin^2(\theta) (\phi')^2} d\theta \quad \left( \begin{array}{l} \text{Could have also} \\ \text{done } \theta = \theta(\phi) \end{array} \right)$$

Integrand independent of  $\phi$ , so via first integral (2.4)

$$\frac{\partial}{\partial \phi'} (\text{integrand}) = \text{const} = k$$

$$\frac{\phi' \sin^2(\theta)}{\sqrt{1 + \sin^2(\theta) (\phi')^2}} = k$$

● Square to obtain

$$(\phi')^2 \sin^4(\theta) = k^2 + k^2 \sin^2(\theta) (\phi')^2$$

$$\Rightarrow \phi' = \pm \frac{k}{\sin \theta \sqrt{\sin^2 \theta - k^2}}$$

$$\Rightarrow \phi - \phi_0 = \pm k \int \frac{1}{\sin \theta \sqrt{\sin^2 \theta - k^2}} d\theta$$

$\pm$  means two possible directions along "great circle"

$\cot \theta = u$  gives

$$\pm \frac{\sqrt{1-k^2}}{k} \cos(\phi - \phi_0) = \cot \theta$$

● Plug  $x$  and  $y$  back in to obtain  $z = \alpha x + \beta y$  for some  $\alpha, \beta \in \mathbb{R}$ , i.e. we indeed have a great circle

L4.2

(ii) Another type of first integral. Assume  $f = f(y, y')$  in (2.3)

i.e.  $\partial f / \partial x = 0$ . Then

Claim  $f - y' \frac{\partial f}{\partial y'} = \text{const}$  (along solution curves) (2.5)

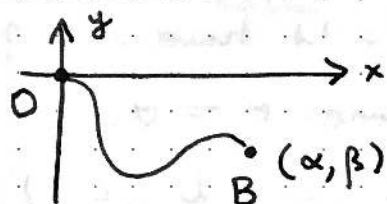
Proof  $\frac{d}{dx} \left( f - y' \frac{\partial f}{\partial y'} \right) = \underbrace{\frac{\partial f}{\partial x}}_{\text{zero}} + y' \frac{\partial f}{\partial y} + \underbrace{y'' \frac{\partial f}{\partial y'} - y'' \frac{\partial f}{\partial y'}}_{\text{zero}} - y' \frac{d}{dx} \left( \frac{\partial f}{\partial y'} \right)$

We are left with

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

which is true by Euler-Lagrange. □

Example The Brachistochrone problem.



Minimize travel time

$$T = \int_A^B dt = \int_A^B \frac{dl}{v(x, y)}$$

$$F[y] = \frac{1}{\sqrt{2g}} \int_0^\beta \underbrace{\frac{\sqrt{1+(y')^2}}{\sqrt{-y}}}_{f(y, y')} dx$$

Using (2.5) we deduce

$$k = f - y' \frac{\partial f}{\partial y'} = \frac{\sqrt{1+(y')^2}}{\sqrt{-y}} - y' \cdot \frac{y'}{\sqrt{-y} \sqrt{1+(y')^2}}$$

$$= \frac{1+(y')^2 - (y')^2}{\sqrt{-y} \sqrt{1+(y')^2}} \quad \Rightarrow \quad (y')^2 + 1 = \frac{1}{-yk^2}$$

$$\Rightarrow y' = \pm \sqrt{\frac{1}{-yk^2} - 1}$$

Integrate to deduce

$$x = \pm k \int \frac{\sqrt{-y}}{\sqrt{1+k^2 y}} dy$$

L4.3

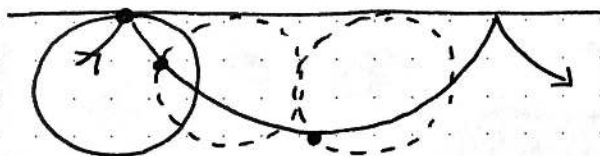
Now let  $y = -\frac{1}{k^2} \sin^2\left(\frac{\theta}{2}\right)$  so that

$$\begin{aligned} x &= \pm k \int \frac{\sin(\theta/2)}{\cos(\theta/2)} \cdot -\frac{1}{k^2} \sin(\theta/2) \cos(\theta/2) d\theta \\ &= \mp \frac{1}{2k^2} (\theta - \sin\theta) + c \end{aligned}$$

Initial conditions  $A = (0, 0) \rightarrow c = 0$

$$\begin{cases} x = \frac{\theta - \sin\theta}{2k^2} \\ y = -\frac{1}{k^2} \sin^2(\theta/2) \end{cases}$$

parametric equations of cycloid  $\odot$



- The curve traced by a point on the rim of a circle, as the circle rolls on a straight line.

Brachistochrone is a cycloid (Bernoulli 1697)

### § 2.2 Fermat's principle

"Light/sound moves along paths which minimise the time of the journey"

Ray ("light")  $y = y(x)$ . Speed of light/sound  $c(x, y)$ .

$$F[y] = \text{Time} = \int_A^B \frac{dl}{c(x, y)} = \int_a^b \frac{\sqrt{1+(y')^2}}{c(x, y)} dx$$

Assume that  $c = c(x)$ .



$$L5.2 \quad A[y] = \int_{\alpha}^{\beta} (y_2(x) - y_1(x)) dx = \oint_C y(x) dx$$

Impose constraint

$$L = \oint \sqrt{1 + y'^2} dx$$

$\lambda$  = Lagrange multiplier

E-L equations on h

$$h(x, y, y', \lambda) = y - \lambda \sqrt{1 + (y')^2}$$

Use 1<sup>st</sup> integral (2.5) to obtain

$$h - y' \frac{\partial h}{\partial y'} = \text{const.} \Rightarrow y - \lambda \sqrt{1 + y'^2} + y' \cdot \frac{\lambda y'}{\sqrt{1 + y'^2}} = \text{const.} = K$$

$$\Rightarrow y - K = \frac{\lambda}{\sqrt{1 + y'^2}} \quad \text{1st order ODE}$$

Solution is

$$(x - x_0)^2 + (y - y_0)^2 = \lambda^2$$

where  $y_0 = K$ .

Circle of radius  $\lambda$ ,

but  $2\pi\lambda = L$

$$\text{so } \lambda = \frac{L}{2\pi}$$

Example The Sturm-Liouville problem

Let  $p(x) > 0$  for  $x \in [\alpha, \beta]$ .

$$\text{Consider } F[y] = \int_{\alpha}^{\beta} [p(x) \cdot (y')^2 + \sigma(x) y^2] dx$$

$$\text{subject to } G[y] = \int_{\alpha}^{\beta} y^2 dx = 1$$

$$h(x, y, y', \lambda) = (p(y')^2 + \sigma y^2) - \lambda \left( y^2 - \frac{1}{\beta - \alpha} \right)$$

$$\text{E-L (3.1): } \frac{\partial h}{\partial y'} = 2p y' \quad \frac{\partial h}{\partial y} = 2\sigma y - 2\lambda y$$

$$\Rightarrow \frac{d}{dx} \left( \frac{\partial h}{\partial y'} \right) = \frac{\partial h}{\partial y} \Rightarrow \boxed{-\frac{d}{dx} (p y') + \sigma y = \lambda y} \quad (3.2)$$

Sturm-Liouville  
eigenvalue problem

$$L(y) = \lambda y \quad \text{where } L = -\frac{d}{dx} (p \cdot) + \sigma$$

Sturm-Liouville  
operator

$\lambda$  is an eigenvalue

L5.3

E.g. If  $p(x) = 1$  and  $\sigma(x) > 0$  "Potential"

obtain the Schrödinger equation with energy  $\lambda$

• If  $\sigma > 0$ , then  $F[y] > 0$

Claim Positive minimum is equal to lowest eigenvalue in (3.2)

Proof Integrate (3.2)  $\times y$  from  $\alpha$  to  $\beta$ :

$$\int_{\alpha}^{\beta} \left( \left[ -\frac{d}{dx} (py') \right] y + \sigma y^2 \right) dx = \lambda \int_{\alpha}^{\beta} y^2 dx$$

Integrate by parts and get  $F[y] = \lambda G[y]$

so  $\lambda_{\min} = F[y] / G[y]$

L6.1

## § 3.2 Several dependant variables

$$(y_1(x), \dots, y_n(x)) = \underline{y}(x)$$

$$F[\underline{y}] = \int_{\alpha}^{\beta} f(x, y_1, \dots, y_n, y_1', \dots, y_n') dx$$

$$\underline{y}(\alpha) = \underline{y}_1 \text{ and } \underline{y}(\beta) = \underline{y}_2$$

Follow the derivation of (2.3):  $\underline{y}(x) \rightarrow \underline{y}(x) + \underline{\eta}(x) \cdot \varepsilon$

Where  $\underline{\eta}(\alpha) = \underline{\eta}(\beta) = 0$ .

$$F[\underline{y} + \varepsilon \underline{\eta}] = F[\underline{y}] + \varepsilon \int_{\alpha}^{\beta} \left( \sum_i \frac{\partial f}{\partial y_i} \eta_i + \frac{\partial f}{\partial y_i'} \eta_i' \right) dx$$

$$- \underbrace{\frac{d}{dx} \left( \frac{\partial f}{\partial y_i'} \right) \eta_i}_{\text{boundary terms}} ] = 0$$

Apply Lemma:

$$\frac{\partial f}{\partial y_i} - \frac{d}{dx} \left( \frac{\partial f}{\partial y_i'} \right) = 0 \text{ for } i=1, \dots, n \quad (3.3)$$

System of  $n$  2<sup>nd</sup> order E-L equations

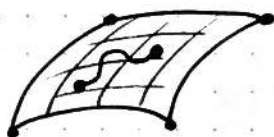
First integrals

$$a) \frac{\partial f}{\partial y_j} = 0 \text{ for } 1 \leq j \leq n \stackrel{(3.3)}{\Rightarrow} \frac{\partial f}{\partial y_j'} = \text{const.}$$

$$b) \frac{\partial f}{\partial x} = 0 \stackrel{(3.3)}{\Rightarrow} f - \sum_{i=1}^n y_i' \frac{\partial f}{\partial y_i'} = \text{const.}$$

Example Geodesics (shortest paths) on a surface

$$\Sigma \subseteq \mathbb{R}^3$$



$$\Sigma \text{ given by } g(\underline{x}) = 0$$

$$\text{Curve } t \rightarrow \underline{x}(t) \quad \begin{array}{l} \underline{x}(\alpha) = \underline{x}_1 \\ \underline{x}(\beta) = \underline{x}_2 \end{array}$$

↑  
indep  
variable

$$\tilde{F}[\underline{x}] = \int_{\alpha}^{\beta} |\underline{x}'(t)| dt \quad \text{but introduce } \lambda(t) \text{ so}$$

$$F[\underline{x}] = \int_{\alpha}^{\beta} [|\underline{x}'(t)| - \lambda(t) g(\underline{x})] dt$$

$$\text{EL with } \lambda \quad \frac{\partial f}{\partial \lambda} - \frac{d}{dx} \left( \frac{\partial f}{\partial \lambda'} \right) = 0 \Rightarrow g(\underline{x}) = 0 \quad \ddot{\phantom{x}}$$

EL with  $\underline{x}$

give geodesic ODEs

### § 3.3 Several independent variables

$$\Phi: \mathbb{R}^3 \rightarrow \mathbb{R} \quad \text{i.e. } \phi(x, y, z)$$

( $\alpha \in \mathbb{R}^n$ )

$$F[\phi] = \int_{D \subseteq \mathbb{R}^3} f(x, y, z, \phi, \phi_x, \phi_y, \phi_z) dx dy dz$$

$\swarrow \frac{\partial \phi}{\partial x}$

Perturb to 1<sup>st</sup> order in  $\epsilon$ :  $\phi \rightarrow \phi + \epsilon \eta(x, y, z)$

$$F[\phi + \epsilon \eta] - F[\phi]$$

$$\eta = 0 \text{ on } \partial D$$

$$= \epsilon \int_D \left( \frac{\partial f}{\partial \phi} \eta + \frac{\partial f}{\partial \phi_x} \eta_x + \text{cyc} \right) dx dy dz$$

$$= \epsilon \int_D \left[ \frac{\partial f}{\partial \phi} - \frac{\partial}{\partial x} \left( \frac{\partial f}{\partial \phi_x} \right) - \text{cyc} \right] \eta dV$$

$\nabla \cdot \left( \frac{\partial f}{\partial \phi_i} \eta \right)$  & use div theorem

Apply Lemma to deduce

$$\frac{\partial f}{\partial \phi} - \sum_{i=1}^3 \frac{\partial}{\partial x_i} \left( \frac{\partial f}{\partial \phi_{x_i}} \right) = 0$$

(3.4)  
PDE

Remains valid for  $\phi: \mathbb{R}^n \rightarrow \mathbb{R}$

Example  $\phi: \mathbb{R}^2 \rightarrow \mathbb{R}$ ,  $\phi(x, y)$

Extremise  $F[\phi] = \int_D \frac{1}{2} (\phi_x^2 + \phi_y^2) dx dy$

$$\frac{\partial f}{\partial \phi} = 0, \quad \frac{\partial f}{\partial \phi_x} = \phi_x, \quad \frac{\partial f}{\partial \phi_y} = \phi_y$$

$$(3.4) \Rightarrow \frac{\partial}{\partial x} \phi_x + \frac{\partial}{\partial y} \phi_y = 0 \Rightarrow \phi_{xx} + \phi_{yy} = 0$$

Example Minimal surfaces



Construct  $\Sigma \subseteq \mathbb{R}^3$  with prescribed boundary and minimal area (soap film)

$$\Sigma = \{ \underline{x} \in \mathbb{R}^3 : g(\underline{x}) = 0 \}$$

write  $\Sigma$  as a graph  $z = \phi(x, y)$



L6.3

$$ds^2 = dx^2 + dy^2 + dz^2 = (1 + \phi_x^2) dx^2 + (1 + \phi_y^2) dy^2 + 2\phi_x \phi_y dx dy$$

Riemannian metric  $\ddot{\circ}$

$$\underbrace{\begin{pmatrix} 1 + \phi_x^2 & \phi_x \phi_y \\ \phi_x \phi_y & 1 + \phi_y^2 \end{pmatrix}}_G$$

Area element

$$\sqrt{\det G} dx dy = \sqrt{1 + \phi_x^2 + \phi_y^2} dx dy$$

$$F[\phi] = \int \sqrt{1 + \phi_x^2 + \phi_y^2} dx dy$$

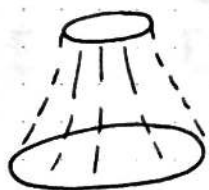
$$\frac{\partial f}{\partial \phi} = 0 \quad \frac{\partial f}{\partial \phi_x} = \frac{\phi_x}{\sqrt{1 + \phi_x^2 + \phi_y^2}} \quad \text{similar for } \frac{\partial f}{\partial \phi_y}$$

Expand (3.4) to obtain

$$(1 + \phi_y^2) \phi_{xx} + (1 + \phi_x^2) \phi_{yy} - 2\phi_x \phi_y \phi_{xy} = 0 \quad (3.5)$$

« Pretty hard »

Assume circular symmetry  $\phi(x, y) = z(r)$



Exercise: (3.5)  $\Rightarrow$  ODE

$$\cancel{z = r_0} \quad r = r_0 \cosh\left(\frac{z - z_0}{r_0}\right)$$

Similarly,  $\mathbb{R}^n$  is not homeomorphic to  $\mathbb{R}^m$  if  $n \neq m$

Homeomorphism  $[0, 1] \times [0, 1] \cong [0, 1] \times [0, 1] \cong [0, 1]$

In fact:  $\mathbb{R}^n \cong \mathbb{R}^m \Leftrightarrow n = m$

For fixed  $X \subseteq (\mathbb{R}^n, \mathcal{O}_X)$  be a topological subspace

Then a loop in  $X$  is a continuous map  $S^1 \rightarrow X$

The set of loops in  $X$ , write

$$\mathcal{L}X = \{f: S^1 \rightarrow X \mid f \text{ continuous}\}$$

is called the free loop space of  $X$ .

In fact,  $\mathcal{L}X$  is a metric or combinatorial space

For any  $n$  and  $m$ ,  $\mathcal{L}(\mathbb{R}^n) \cong \mathcal{L}(\mathbb{R}^m)$



L7.2

Claim this is a minimum of  $F$ .

$$F[y+\eta] - F[y] = \int_0^1 [(y''+\eta'')^2 - (y'')^2] dx$$

$$= \int_0^1 [(\eta'')^2 + 2(\eta'')(y'')] dx$$

$$= \underbrace{\int_0^1 (\eta'')^2 dx}_{> 0 \text{ if } \eta \neq 0} + 2 \underbrace{\int_0^1 (\eta'')(y'')}_{\frac{d}{dx}(\eta' y'') - \eta' y''}$$

> 0 if  $\eta \neq 0$

$$\frac{d}{dx}(\eta' y'')$$

↑  
gives 0

$$-\eta' y'' = \frac{d}{dx}(6\eta)$$

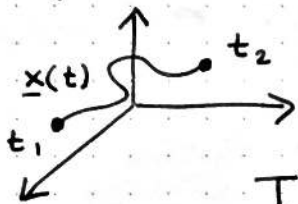
↑  
gives 0

$$\therefore F[y+\eta] > F[y] \quad \ddot{\circ}$$

## §4 Least action principle and Noether's theorem

### §4.1 Variational formulation of dynamics

A particle of unit mass moves in  $\mathbb{R}^3$ .



$t =$  independent variable

3 dependent variables

$T =$  kinetic energy

$V =$  potential energy

$$L = T - V = \text{Lagrangian} \quad (4.1)$$

$$S[\underline{x}] = \int_{t_1}^{t_2} L dt = \text{action} \quad (4.2)$$

Hamilton's principle (aka "Least action principle"):

The action is stationary along the path taken

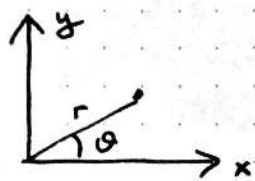
So  $L$  satisfies the E-L equations

Example  $T = \frac{1}{2} |\dot{\underline{x}}|^2$ ,  $V = V(\underline{x})$

$$\frac{\partial L}{\partial \dot{x}_i} = \dot{x}_i, \quad \frac{\partial L}{\partial x_i} = -\frac{dV}{dx_i}$$

L7.3  
 E-L eq<sup>n</sup>  $\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}_i} \right) = \frac{\partial L}{\partial x_i} \Rightarrow \ddot{x}_i = -\nabla V$  (Newton)

● Example particle in  $\mathbb{R}^2$  moving in radial potential



$$L = \frac{1}{2} (\dot{r}^2 + r^2 \dot{\theta}^2) - V(r)$$

E-L eq<sup>n</sup>  $\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{r}} \right) - \frac{\partial L}{\partial r} = 0$

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{\theta}} \right) - \frac{\partial L}{\partial \theta} = 0$$

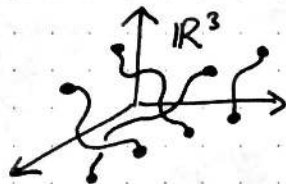
explore first integrals

$$\frac{\partial L}{\partial \theta} = 0 \Rightarrow \frac{\partial L}{\partial \dot{\theta}} = r^2 \dot{\theta} = \text{const.} \quad \dot{\theta}$$

$$\frac{\partial L}{\partial t} = 0 \Rightarrow \dot{\theta} \frac{\partial L}{\partial \dot{\theta}} + \dot{r} \frac{\partial L}{\partial \dot{r}} - L = \underbrace{\frac{1}{2} (\dot{r}^2 + r^2 \dot{\theta}^2) + V(r)}_{\text{Energy } \ddot{u}}$$

is constant as well

Example (Configuration space)



Consider  $N$  particles in  $\mathbb{R}^3$

$\underline{x}_1, \dots, \underline{x}_N$  positions

Work in  $C = \mathbb{R}^{3N}$  where  $q \in C$  has

$(q_1^1, q_2^1, q_3^1, \dots, q_3^N)$  as the components of the particles

$N$  paths in  $\mathbb{R}^3 \rightarrow 1$  path in  $C$

Now  $L = L(\underset{\substack{\uparrow \\ \text{dependent}}}{q^i}, \underset{\substack{\uparrow \\ \text{indep}}}{\dot{q}^i}, t)$  and  $S[q] = \int_{t_1}^{t_2} L dt.$

## §4.2 Noether's theorem

$$\bullet F[\underline{q}] = \int_{t_1}^{t_2} L(q^i, \dot{q}^i, t) dt$$

Example  $L = \frac{1}{2}(\dot{q}^i \dot{q}^i) - V(q^1 - q^2)$

$$Q^1 = -q^2, Q^2 = -q^1 \Rightarrow L(Q^1, Q^2, \dot{Q}^1, \dot{Q}^2) = L(q^1, q^2, \dot{q}^1, \dot{q}^2)$$

This is a symmetry of  $L$ , albeit a discrete symmetry.

Instead take  $Q^1 = q^1 + s, Q^2 = q^2 + s, s \in \mathbb{R}$

Also a symmetry for any  $s$ , so have a continuous symmetry.

In general, a continuous symmetry of  $L$  is a 1-parameter family of transformations  $q^i(t) \rightarrow Q^i(s, t)$  such that

$$\bullet Q^i(0, t) = q^i(t), Q^i \text{ is } C^1 \text{ in } s, \text{ and}$$

$$L(Q^i, \dot{Q}^i, t) = L(q^i, \dot{q}^i, t) \quad \forall s$$

Theorem Given a continuous symmetry of  $L$ ,

$$\sum_i \frac{\partial L}{\partial \dot{q}^i} \frac{\partial Q^i}{\partial s} \Big|_{s=0} \text{ is a 1st integral of the E-L equations.} \quad (4.3)$$

Proof  $0 = \frac{d}{ds} L(Q^i(s, t), \dot{Q}^i(s, t), t) \Big|_{s=0}$

$$= \left( \frac{\partial L}{\partial Q^i} \frac{\partial Q^i}{\partial s} + \frac{\partial L}{\partial \dot{Q}^i} \frac{\partial \dot{Q}^i}{\partial s} \right) \Big|_{s=0}$$

$$\bullet \stackrel{\text{E-L}}{=} \left( \frac{d}{dt} \frac{\partial L}{\partial \dot{q}^i} \right) \frac{\partial Q^i}{\partial s} + \frac{\partial L}{\partial \dot{q}^i} \frac{d}{dt} \left( \frac{\partial Q^i}{\partial s} \right) \Big|_{s=0}$$

$$= \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}^i} \frac{\partial Q^i}{\partial s} \right) \text{ as desired} \quad \square$$

Back to the example,

$$\frac{\partial Q^i}{\partial s} \Big|_{s=0} = 1, \quad \frac{\partial L}{\partial \dot{q}^i} = \dot{q}^i$$

$$\Rightarrow \dot{q}_1 + \dot{q}_2 \text{ is a 1st integral} \quad * \quad (\text{momentum})$$

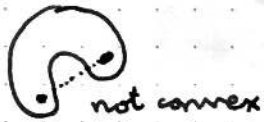
L7.2

## §5 Convex functions

Go back to calculus in  $\mathbb{R}^n$ . Study a class of functions where finding min/max is easy.

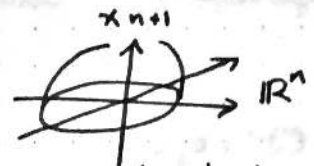
Def<sup>n</sup> a) A set  $S \subseteq \mathbb{R}^n$  is convex if

$$\forall \underline{x}, \underline{y} \in S, t \in [0,1], (1-t)\underline{x} + t\underline{y} \in S$$



b) A graph of a function  $f: \mathbb{R}^n \rightarrow \mathbb{R}$  is a surface  $\Sigma$  in  $\mathbb{R}^{n+1}$  given by  $x_{n+1} - f(x_1, \dots, x_n) = 0$ .

E.g.  $f(\underline{x}) = \sqrt{1 - |\underline{x}|^2}$  gives a hemisphere

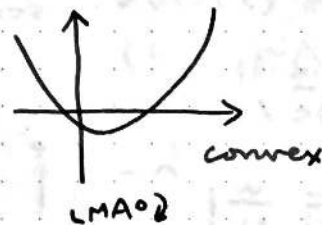
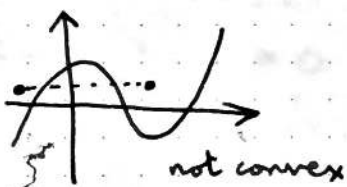


c) A chord of  $f: \mathbb{R}^n \rightarrow \mathbb{R}$  is a straight line segment between two points on the graph of  $f$ .

Def<sup>n</sup> A function  $f: \mathbb{R}^n \rightarrow \mathbb{R}$  is convex if

$$f((1-t)\underline{x} + t\underline{y}) \leq (1-t)f(\underline{x}) + tf(\underline{y}) \quad (5.1) \quad \Leftrightarrow \text{convex epigraph}$$

$$\forall \underline{x}, \underline{y} \in \mathbb{R}^n, t \in [0,1]$$



Note 1)  $f$  is concave if  $-f$  is convex, i.e. (5.1) has  $\geq$

2)  $f$  is strictly convex if for  $t \in (0,1)$ ,  $\underline{x} \neq \underline{y}$ , (5.1) has  $<$

Example  $f: \mathbb{R} \rightarrow \mathbb{R}$ ,  $f(x) = x^2$

$$f((1-t)x + ty) - (1-t)f(x) - tf(y)$$

$$= (1-t)^2 x^2 + 2t(1-t)xy + t^2 y^2 - (1-t)x^2 - ty^2$$

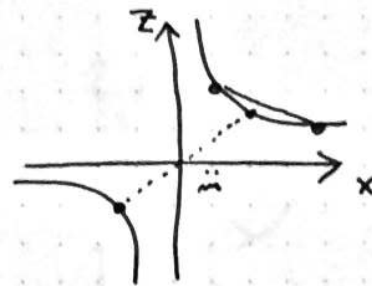
$$= -t(1-t)x^2 - t(1-t)y^2 + 2t(1-t)xy$$

$$= -t(1-t)(x-y)^2 < 0 \text{ for } t \in (0,1), x \neq y$$

So  $f$  is strictly convex

L8.3

Example  $f: \mathbb{R} \setminus \{0\} \rightarrow \mathbb{R}, f(x) = 1/x$



●  $f$  not convex

But  $f|_{\mathbb{R}_+}$  is convex

### § 5.1 Conditions for convexity

3 different tests for convexity

a) If  $f$  is once diff'ble, then  $f$  is convex iff  $\forall \underline{x}, \underline{y}$

$$f(\underline{y}) \geq f(\underline{x}) + (\underline{y} - \underline{x}) \cdot \nabla f(\underline{x}) \quad (5.2)$$

Proof 1) Assuming (5.2), have that  $\forall \underline{x}, \underline{y}, \underline{z}$

$$f(\underline{x}) \geq f(\underline{z}) + (\underline{x} - \underline{z}) \cdot \nabla f(\underline{z})$$

$$\bullet f(\underline{y}) \geq f(\underline{z}) + (\underline{y} - \underline{z}) \cdot \nabla f(\underline{z})$$

1.  $(1-t) + 2 \cdot t$  gives

$$(1-t)f(\underline{x}) + tf(\underline{y}) \geq f(\underline{z}) + [(1-t)\underline{x} + t\underline{y} - \underline{z}] \cdot \nabla f(\underline{z})$$

Take  $\underline{z} = (1-t)\underline{x} + t\underline{y}$  and be done.

" $\Rightarrow \square$ "

2) Conversely, assume (5.1) and define, for  $\underline{x}, \underline{y}$  fixed,

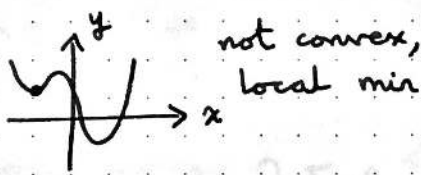
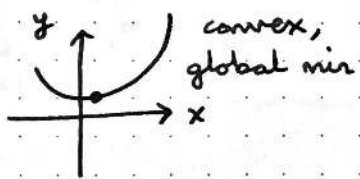
$$h(t) = (1-t)f(\underline{x}) + tf(\underline{y}) - f((1-t)\underline{x} + t\underline{y}) \geq 0 \quad \text{on } [0,1]$$

At  $t=0, h(t)=0 \Rightarrow h'(t) \geq 0$  by diff'bility? yes!

Then obtain  $-f(\underline{x}) + f(\underline{y}) - (\underline{y} - \underline{x}) \cdot \nabla f(\underline{x}) \geq 0$ , as desired.

" $\Leftarrow \square$ "

Claim If  $\underline{x}_0$  is a stationary point of a convex function, then it is an absolute minimum of the function



Proof Follows directly from (5.2)  $f(\underline{y}) \geq f(\underline{x}) + (\underline{y} - \underline{x}) \cdot \nabla f(\underline{x})$   $\square$

b) Another 1st order test.  $f: \mathbb{R}^n \rightarrow \mathbb{R}$  is convex iff

$$(\underline{y} - \underline{x}) \cdot (\nabla f(\underline{y}) - \nabla f(\underline{x})) \geq 0 \quad [\text{Exercise}] \quad (5.3)$$

c) Second order test. Assume  $f$  is a  $C^2$  function  $\mathbb{R}^n \rightarrow \mathbb{R}$ .

Then  $f$  is convex iff all eigenvalues of the Hessian matrix

$$H_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j} \text{ are non-negative } \forall \underline{x} \in \mathbb{R}^n.$$

[If evals strictly positive,  $f$  is strictly convex]

Proof Assume  $f$  is convex, use (5.2) with  $\underline{y} = \underline{x} + \underline{h}$ .

$$f(\underline{x} + \underline{h}) \geq f(\underline{x}) + \underline{h} \cdot \nabla f(\underline{x})$$

$$\text{Expand LHS: } f(\underline{x} + \underline{h}) = f(\underline{x}) + \underline{h} \cdot \nabla f(\underline{x}) + \frac{1}{2} h_i h_j H_{ij}(\underline{x}) + o(h^2)$$

$$\text{We deduce } \frac{1}{2} h_i h_j H_{ij}(\underline{x}) + o(h^2) \geq 0$$

This implies evals of  $H_{ij}$  are all non-negative.

" $\Leftarrow$ " See Townsend's notes

Example  $f: \mathbb{R}_+^2 \rightarrow \mathbb{R}$

$$(x, y) \rightarrow \frac{1}{xy}$$

$$H_{ij} = \frac{1}{xy} \begin{pmatrix} 2/x^2 & 1/xy \\ 1/xy & 2/y^2 \end{pmatrix}$$

$$\text{Determinant } \frac{3}{x^3 y^3} > 0$$

$$\text{Trace } > 0$$

} So  $f$  is strictly convex

## § 6 Legendre transform

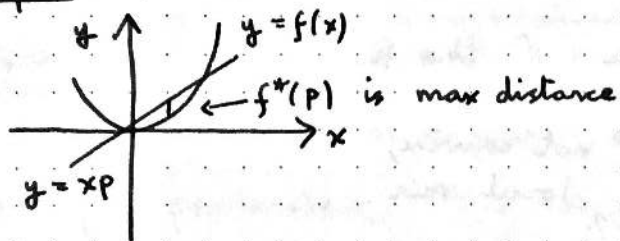
Def<sup>n</sup> The Legendre transform of  $f: \mathbb{R}^n \rightarrow \mathbb{R}$  is

$$f^*(\underline{p}) = \sup_{\underline{x} \in \mathbb{R}^n} (\underline{p} \cdot \underline{x} - f(\underline{x})) \quad (6.1)$$

The domain of  $f^*$  are all  $\underline{p}$  such that the sup exists



Example

 $n=1$ 

$$\frac{\partial}{\partial x} (px - f(x)) = 0$$

gives  $x_0$  s.t.

$$p = \left. \frac{\partial f}{\partial x} \right|_{x_0}$$

Find  $x(p)$  and substitute in (6.1)Take  $f(x) = ax^2$  with  $a > 0$ .

$$\frac{\partial}{\partial x} (px - ax^2) = 0 \Rightarrow p = 2ax, \quad x = \frac{p}{2a}$$

$$\therefore f^*(p) = p \cdot \frac{p}{2a} - a \cdot \frac{p^2}{4a^2} = \frac{p^2}{4a}$$

$$f^{**}(x) = \frac{x^2}{4 \left( \frac{1}{4a} \right)} = ax^2 \quad \circ$$

Relation holds  $\forall$  strictly convex functions  $f$ Note that if  $a < 0$ ,  $f^*$  undefined everywhereProp Legendre transforms are convex functions with convex domain  $\Leftarrow$ 

$$\text{Proof } f^*((1-t)\underline{p} + t\underline{q}) = \sup_{\underline{x} \in \mathbb{R}^n} ((1-t)\underline{p} \cdot \underline{x} + t\underline{q} \cdot \underline{x} - f(\underline{x}))$$

$$= \sup_{\underline{x} \in \mathbb{R}^n} ((1-t)\underline{p} \cdot \underline{x} + t\underline{q} \cdot \underline{x} - f(\underline{x}) + tf(\underline{x}) - tf(\underline{x}))$$

$$= \sup_{\underline{x} \in \mathbb{R}^n} ((1-t)\underline{p} \cdot \underline{x} - (1-t)f(\underline{x}) + t\underline{q} \cdot \underline{x} - tf(\underline{x}))$$

$$\leq (1-t) \sup_{\underline{x} \in \mathbb{R}^n} (\underline{p} \cdot \underline{x} - f(\underline{x})) + t \sup_{\underline{x} \in \mathbb{R}^n} (\underline{q} \cdot \underline{x} - f(\underline{x}))$$

$$= (1-t)f^*(\underline{p}) + tf^*(\underline{q})$$

This shows  $f^*$  defined on a convex set, and is convex.  $\square$ How to find  $f^*$  in practice? Assume  $f$  is strictly convex, diff'bleTo find sup in (6.1),  $\nabla(\underline{p} \cdot \underline{x} - f(\underline{x})) = 0 \Rightarrow \underline{p} = \nabla f(\underline{x})$ Now if  $f$  strictly convex, can invert for  $\underline{x}(\underline{p})$ Substitute back to yield  $f^*(\underline{p}) = \underline{p} \cdot \underline{x}(\underline{p}) - f(\underline{x}(\underline{p}))$ It is true that  $f^{**} = f$  (No proof given) for  $f$  strictly convex

§ 6.1 Applications in thermodynamics

\* Durajski not like how this is presented \*

Complex system, like a gas, can be described in terms of a few macroscopic parameters,  $T = \text{temperature}$ ,  $V = \text{volume}$

$p = \text{pressure}$ ,  $S = \text{entropy}$

Internal energy  $U(S, V)$  satisfies 1<sup>st</sup> law of thermo:

$$dU = T dS - p dV$$

L10.1

$$U(S, V) \text{ and } dU = TdS - pdV$$

$$\begin{aligned} \text{Free energy } F &= \min_S (U - TS) = F(T, V) \\ &= - \max_S (TS - U) = -U^*(T) \end{aligned}$$

Legendre transform wrt  $S$  regarding  $V$  as a parameter

$$\frac{\partial}{\partial S} (TS - U) \Big|_V = 0 \Rightarrow T = \frac{\partial U}{\partial S} \Big|_V$$

$$\begin{aligned} \text{Enthalpy } H(p, S) &= \min_V (U + PV) \\ &= - \max_V ((-p)V - U) = -U^*(-p) \end{aligned}$$

Legendre transform wrt  $V$

$$\frac{\partial}{\partial V} (U + pV) \Big|_S = 0 \Rightarrow p = - \frac{\partial U}{\partial V} \Big|_S$$

In both cases Legendre transform swaps roles of thermodynamic quantities:

$$\begin{array}{ccc} U(S, V) & \xrightarrow{S} & F(T, V) \\ \downarrow V & \nearrow & \\ H(p, S) & & \end{array}$$

## § 7 Hamiltonian mechanics

Recall (§4.1) the Lagrangian  $L(q^i, \dot{q}^i, t) = T - V$

$q^i$  = "positions"     $v^i = \dot{q}^i$  = "velocities"

$H$  = Legendre transform of  $L$  wrt the velocities

$$H(p_i, q^i, t) = \sup_{\underline{v}} (p_i v^i - L(q^i, v^i, t))$$

$$p_i = \frac{\partial L}{\partial v_i} \text{ at sup } \Rightarrow \text{invert relation}$$

$$H = p_i v^i(\underline{p}, \underline{q}) - L(\underline{q}, \underline{v}(\underline{p}, \underline{q}), t) \quad (7.1)$$

$$\text{Example } L = m \frac{|\underline{v}|^2}{2} - V(\underline{q}) \quad p_i = \frac{\partial L}{\partial v_i} = m v_i$$

$$\therefore H(\underline{p}, \underline{q}, t) = - \frac{m}{2} \frac{|\underline{p}|^2}{m^2} + V(\underline{q}) = \frac{|\underline{p}|^2}{2m} + V(\underline{q})$$

$$+ \underline{p} \cdot \frac{\underline{p}}{m}$$

$\underline{p}$  = momenta

$\dot{\circ}$   
total energy

What about E-L equations?

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{v}^i} \right) = \frac{\partial L}{\partial q^i}$$

Compute  $dH$  in two ways.

$$dH = \frac{\partial H}{\partial p_i} dp_i + \frac{\partial H}{\partial q^i} dq^i + \frac{\partial H}{\partial t} dt$$

$$= d(p_i \dot{q}^i - L(q^i, \dot{q}^i, t))$$

$$= \dot{q}^i dp_i + \underbrace{p_i}_{\substack{\downarrow \\ \dot{p}_i \text{ by E-L}}} d\dot{q}^i - \frac{\partial L}{\partial q^i} dq^i - \underbrace{\left[ \frac{\partial L}{\partial \dot{q}^i} \right]}_{= p_i} d\dot{q}^i - \frac{\partial L}{\partial t} dt$$

$$= \dot{q}^i dp_i - p_i d\dot{q}^i - \frac{\partial L}{\partial t} dt$$

Now compare coeffs to deduce

$$\dot{q}^i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q^i}, \quad \frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t} \quad (7.2)$$

Hamilton's equations

$2n$  first order ODEs

↑ note  $\frac{\partial}{\partial t}$  means different

$\exists$  unique solution once  $p_i, q^i$  at  $t=0$  are specified

initial data  $\rightarrow p_i(t), q^i(t)$  is a curve in  $2n$ -dimensional phase space

Hamiltonian formulation links with quantum dynamics (PQM)

Example Take  $n=1$ ,  $H(p, q) = \frac{p^2}{2m} + V(q)$

$$(7.2) \rightarrow \dot{q} = \frac{\partial H}{\partial p} = \frac{p}{m}, \quad \dot{p} = -\frac{\partial H}{\partial q} = -V'$$

$$\downarrow p = m\dot{q} \quad \rightarrow \quad m\ddot{q} = -V' \quad \text{ö N2}$$

Hamilton's equations from the least action principle

$$L = \underline{p} \cdot \underline{\dot{q}} - H(\underline{p}, \underline{q}, t) \quad \text{where ...}$$

$$S[\underline{p}, \underline{q}, t] = \int_{t_1}^{t_2} \underbrace{(p_i \dot{q}^i - H(p, q, t))}_{\text{L}} dt$$

E-L equations for  $2n$  dependant variables  $\underline{q}, \underline{p}$

$$\frac{\partial f}{\partial q^i} = \frac{d}{dt} \left( \frac{\partial f}{\partial \dot{q}^i} \right), \quad \frac{\partial f}{\partial p_i} = \frac{d}{dt} \left( \frac{\partial f}{\partial \dot{p}_i} \right)$$

↑ zero

L10.3

$$\text{So } \dot{q}_i - \frac{\partial H}{\partial p_i} = 0.$$

Other eq<sup>n</sup>s give

$$-\frac{\partial H}{\partial q_i} = \frac{d}{dt} p_i$$

} gives (7.2)

sh boy

§8 The second variation

Look at the nature of stationary points of a functional (2.1)

$$F[y] = \int_{\alpha}^{\beta} f(x, y, y') dx \quad y \rightarrow y + \epsilon \eta(x) \text{ s.t. } \eta(\alpha) = \eta(\beta) = 0$$

$$F[y + \epsilon \eta] - F[y] = \int_{\alpha}^{\beta} [f(x + \epsilon \eta, y + \epsilon \eta, y' + \epsilon \eta') - f(x, y, y')] dx$$

Expand in  $\epsilon$  up to quadratic terms. Assume  $y(x)$  satisfies E-L

$$F[y + \epsilon \eta] - F[y] = \underbrace{\epsilon \int_{\alpha}^{\beta} \eta \left( \frac{\partial f}{\partial y} - \frac{d}{dx} \left( \frac{\partial f}{\partial y'} \right) \right) dx}_{\text{zero by E-L}} + \frac{1}{2} \epsilon^2 \int_{\alpha}^{\beta} \left\{ \eta^2 \frac{\partial^2 f}{\partial y^2} + 2\eta \eta' \frac{\partial^2 f}{\partial y \partial y'} + \eta'^2 \frac{\partial^2 f}{\partial y'^2} \right\} dx + o(\epsilon^2)$$

Note  $2 \frac{\partial^2 f}{\partial y \partial y'} \eta \eta' = \frac{\partial^2 f}{\partial y \partial y'} \frac{d}{dx} (\eta^2) = \frac{d}{dx} \left( \frac{\partial^2 f}{\partial y \partial y'} \eta^2 \right) - \eta^2 \frac{d}{dx} \left( \frac{\partial^2 f}{\partial y \partial y'} \right)$

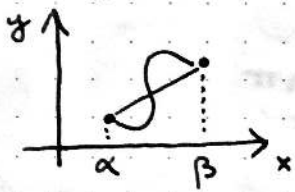
$$\delta^2 F[y] = \frac{1}{2} \int_{\alpha}^{\beta} (Q \eta^2 + P(\eta')^2) dx \quad \left. \begin{array}{l} \text{the second} \\ \text{variation} \end{array} \right\} \begin{array}{l} (8.1) \\ \text{vanishes} \\ \text{on integration} \end{array}$$

$$P = \frac{\partial^2 f}{\partial y'^2} \quad Q = \frac{\partial^2 f}{\partial y^2} - \frac{d}{dx} \left( \frac{\partial^2 f}{\partial y \partial y'} \right)$$

We proved

Prop If  $y(x)$  is a solution to the E-L equation, and if  $Q \eta^2 + P(\eta')^2 > 0 \quad \forall \eta$  s.t.  $\eta(\alpha) = \eta(\beta) = 0$  [and  $P, Q$  as in 8.1] then  $y(x)$  is a local minimiser of (2.1)

Example geodesics on  $\mathbb{R}^2$



$$F[y] = \int_{\alpha}^{\beta} \sqrt{1 + (y')^2} dx$$

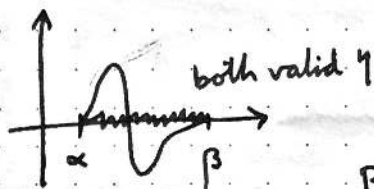
$$Q = 0, \quad P = \frac{\partial^2 f}{\partial y'^2} = \frac{\partial}{\partial y'} \left( \frac{y'}{\sqrt{1 + (y')^2}} \right) = \frac{1}{(1 + (y')^2)^{3/2}} > 0$$

It follows that  $\int P(\eta')^2 > 0$  for all non-zero  $\eta$

Go back to (8.1)

Prop If  $y_0(x)$  is a solution to E-L, then  $P = \frac{\partial^2 f}{\partial y'^2} \geq 0$  (8.2) is a necessary condition for  $y_0$  to be a local minimum

"P is more important than Q"



Proof Assume that  $\exists x_0 \in (\alpha, \beta)$  s.t.  $P < 0$

By continuity  $\exists \delta > 0$  s.t.  $P < -\epsilon/2$  on  $(x_0 - \delta, x_0 + \delta)$

Take  $\eta$  s.t.  $\eta = 0$  outside  $(x_0 - \delta, x_0 + \delta)$  and is small but oscillates rapidly inside  $(x_0 - \delta, x_0 + \delta)$ . (See Gelfand-Fomin for details)

For this choice of  $\eta$ , second variation becomes

$$\delta^2 F[\eta] = \int_{x_0 - \delta}^{x_0 + \delta} \left( \underbrace{-\frac{\epsilon}{2}}_{\text{large}} (\eta')^2 + \underbrace{Q\eta^2}_{\text{bounded}} \right) dx < 0$$

### § 8.1 Associated eigenvalue problem

Try to see if condition  $P > 0$  is sufficient for  $\delta^2 F[\eta] > 0$

Look at (8.1)

$$Q\eta^2 + P\eta'^2 = Q\eta^2 + \frac{d}{dx}(P\eta'\eta) - \underbrace{(P\eta')'}_{\substack{\uparrow \\ \text{vanishes} \\ \text{on } \int}} \eta$$

$$\begin{aligned} \text{So } \delta^2 F[\eta] &= \int_{\alpha}^{\beta} \eta (-P\eta')' + Q\eta \, dx \\ &= \frac{1}{2} \int_{\alpha}^{\beta} \eta \cdot \mathcal{L}(\eta) \, dx \quad (8. \pi) \end{aligned}$$

where  $\mathcal{L}(\eta) = -(P\eta')' + Q\eta$  is the Sturm-Liouville operator

$$\text{If } \exists \eta \text{ s.t. } \begin{cases} \mathcal{L}(\eta) = -\omega^2 \eta & (\omega \text{ real, } \neq 0) \\ \eta(\alpha) = \eta(\beta) = 0 \end{cases} \quad (8.4)$$

then  $\eta$  cannot be a local minimiser, as then

$$\delta^2 F[\eta] = \int_{\alpha}^{\beta} -\omega^2 \eta^2 < 0 \quad \text{if } \eta \neq 0$$

Example Take  $f(y) = \frac{1}{2}[(y')^2 - (y^2)]$ ,  $\alpha = 0$ ,  $\beta \neq n\pi$

Minimise (2.1) subject to  $y(0) = y(\beta) = 0$   $\downarrow$  no sin'n

E-L equations  $y'' + y = 0 \rightarrow y = 0$  is solution

Is this a local minimiser?

$$\delta^2 F[\eta] = \frac{1}{2} \int_0^{\beta} \{ \eta'^2 - \eta^2 \} dx \quad P=1, Q=-1$$

L12.1

$$+ \eta'' + \eta = + \omega^2 \eta \quad \eta = A \sin\left(\frac{\pi x}{\beta}\right) \quad \text{so } \eta(0) = \eta(\beta) = 0$$

$$-\left(\frac{\pi}{\beta}\right)^2 + 1 = \omega^2 \Leftrightarrow 1 - \omega^2 = \left(\frac{\pi}{\beta}\right)^2 \quad \text{P06!} \quad \text{This gets you here if } \beta > \pi$$

In general, problems may arise if  $[\alpha, \beta]$  is ~~too large~~

We shall now make this precise

[Remark: Compare (3.2) The minimum of  $\delta^2 F[y=y_0, \eta]$  as a functional of  $\eta$  is the lowest eigenvalue of  $L$ ]

### § 8.2 Jacobi condition

Legendre tried (and failed) to prove that  $P > 0$  is sufficient for positivity of  $\delta^2 F$ . His idea:

Take any  $\phi \in C^1[\alpha, \beta]$ . Then

$$\int_{\alpha}^{\beta} (\phi \eta^2)' dx = \int_{\alpha}^{\beta} (\phi' \eta^2 + 2\phi \eta \eta') dx$$

↑  
zero  $\forall \phi$

Add this to (8.1) to obtain

$$\begin{aligned} \delta^2 F[y, \eta] &= \int_{\alpha}^{\beta} (P \eta'^2 + 2\phi \eta \eta' + Q \eta^2 + \phi' \eta^2) dx \\ &= \int_{\alpha}^{\beta} \left( \underbrace{P \left( \eta' + \frac{\phi \eta}{P} \right)^2}_{> 0} + \underbrace{\left( Q + \phi' - \frac{\phi^2}{P} \right)}_{\text{take } \phi \text{ s.t. this vanishes}} \eta^2 \right) dx \end{aligned}$$

$$\phi^2 = P(Q + \dots) \sim \text{Riccati type equation} \quad (8.5)$$

Transform into 2<sup>nd</sup> order linear ode:  $\phi = -\frac{P u'}{u}$   $\leftarrow$  need  $u \neq 0$

$$\left( P \left( \frac{u'}{u} \right)^2 \right)' = P \left( Q - P' \frac{u'}{u} - P \frac{u'' u - (u')^2}{u^2} \right)$$

$$Q - P' \frac{u'}{u} - P \frac{u''}{u} = 0 \Rightarrow -(Pu')' + Qu = 0 \quad (8.6)$$

Jacobi's accessory equation

Need solution to (8.6) which is non-zero on  $[\alpha, \beta]$

Such solution could not exist if  $[\alpha, \beta]$  is too large



L12.2

Go back to  $P=1, Q=-1$ . Then (8.6) is

$$u'' + u = 0 \rightarrow u = A \sin(x - x_0) \text{ so rekt for large } \epsilon$$

So  $\ddot{\theta}$