## Extremising Functions (Hessian and Lagrange Multipliers) 1

For a suitably differentiable function  $f : \mathbb{R}^n \to \mathbb{R}$ , the point  $\mathbf{a} \in \mathbb{R}^n$  is stationary if  $\nabla f(\mathbf{a}) = \mathbf{0}$ . The Hessian matrix is given by  $H_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j}$ . The Hessian evaluated at  $\mathbf{x} = \mathbf{a}$  can be used to determine the nature of the stationary point:

- all eigenvalues positive: (local) minimum
- all eigenvalues negative: (local) maximum
- some positive, some negative: saddle
- · some eigenvalue zero: may need higher derivatives

In  $\mathbb{R}^2$ , can determine this purely from the signs of the determinant and trace.

Use Lagrange multipliers to extremise functions subject to constraints, e.g. extremise f(x, y) subject to g(x, y) =0, then consider  $h(x, y, \lambda) = f(x, y) - \lambda g(x, y)$  and extremise h with respect to x, y and  $\lambda$ . Can generalise this for multiple constraints: use more multiplers  $\lambda_i$ . Can also use Lagrange multipliers with integrals (and then use Euler-Lagrange on the combined function).

## 2 Extremising Integrals (Euler-Lagrange)

Seek to extremise a functional  $F[y] = \int_a^b f(x, y, y') dx$ , where y(a) and y(b) are given. Perturb  $y(x) \to y(x) + \epsilon \eta(x)$  with  $\eta(a) = \eta(b) = 0$ . Consider expansion in  $\epsilon$  and write  $F[y + \epsilon \eta] = f[y] + \epsilon \, \delta F + \epsilon^2 \, \delta^2 F + \mathcal{O}(\epsilon^3)$ . Start with the first variation  $\delta F$ , integrating the  $\eta'$  term by parts to reach the form  $\int [\ldots] \eta \, dx$ :

$$\delta F = \int_{a}^{b} \frac{\partial f}{\partial y} \eta + \frac{\partial f}{\partial y'} \eta' dx = \int_{a}^{b} \left[ \frac{\partial f}{\partial y} - \frac{d}{dx} \left( \frac{\partial f}{\partial y'} \right) \right] \eta \, dx$$

For y to make F stationary,  $\delta F$  must be zero for all possible  $\eta(x)$ , hence the square bracket must be zero, yielding the Euler-Lagrange equation:

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

This can be extended in various ways for more general f:

- If more y<sub>i</sub>: there is an E-L equation for each i: d/dx (∂f/∂y'<sub>i</sub>) ∂f/∂y<sub>i</sub> = 0
  If more x<sub>i</sub>: then first term becomes a sum (∑<sub>i</sub> ∂/∂x<sub>i</sub> ∂f/∂y<sub>x<sub>i</sub></sub>)
- If more derivates (e.g. f(x, y, y', y''), then additional terms:  $\dots \frac{d^2}{dx^2} \left( \frac{\partial f}{\partial y''} \right) + \frac{d}{dx} \left( \frac{\partial f}{\partial y'} \right) \frac{\partial f}{\partial y} = 0$

There are two first integrals of Euler-Lagrange for special f:

- If \$\frac{\partial f}{\partial y}\$ = 0: \$\frac{\partial f}{\partial y'}\$ = const (this one is immediate)
  If \$\frac{\partial f}{\partial x}\$ = 0: \$f y' \$\frac{\partial f}{\partial y'}\$ = const: show this by considering \$\frac{df}{dx}\$

To (possibly) determine the nature of a stationary y(x), consider the second variation (coefficient of  $\epsilon^2$ ):

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$$\delta^2 F = \frac{1}{2} \int_a^b Q \eta^2 + P \eta'^2 dx \quad \text{where} \quad Q(x) = \frac{\partial^2 f}{\partial y^2} - \frac{d}{dx} \frac{\partial^2 f}{\partial y \partial y'}, \quad P(x) = \frac{\partial^2 f}{\partial y'^2}$$

where P(x) and Q(x) are evaluated for the stationary y(x). If this is positive for all suitable non-zero  $\eta(x)$ , then y(x) is a local minimum (similarly negative for maximum, and mixed for saddle). Have various partial results:

- (Necessary condition; Legendre condition) if y(x) is a local minimum then  $P(x) \ge 0$  for all x
- (Sufficient condition) P(x) > 0 and Q(x) > 0 for all x: is *sufficient* for y(x) to be a local minimum. Can relax this a little for P and Q to have some zeros, so long as integral for δ<sup>2</sup>F is always positive for any suitable non-zero η(x).
- (Associated eigenvalue problem) define  $\mathcal{L}$  as  $\mathcal{L}\eta = -(P\eta')' + Q\eta$ , and hence  $\delta^2 F = \frac{1}{2} \int \eta[\mathcal{L}\eta] dx$ . The signs of the eigenvalues of  $\mathcal{L}\eta = \lambda \eta$  (with  $\eta = 0$  at the ends) can be used to analogously to the Hessian (all positive for a minimum).
- (Jacobi condition) If there is a u(x) on [a, b] satisfying  $\mathcal{L}u = 0$  and  $u(x) \neq 0$  for any x, then y(x) is a minimiser. This comes from completing the square in the integrand, in essence:

$$\int P\eta'^2 + Q\eta^2 dx = \int P\left(\eta' - \frac{u'}{u}\eta\right)^2 + \frac{\mathcal{L}u}{u}dx$$

## 3 Convexity and Legendre transforms

A set S is convex if  $(1-t)\mathbf{x} + t\mathbf{y} \in S$  for all  $\mathbf{x}, \mathbf{y} \in S$  and for  $0 \le t \le 1$ .

A function f is convex if its domain is a convex set and  $f((1-t)\mathbf{x} + t\mathbf{y}) \le (1-t)f(\mathbf{x}) + tf(\mathbf{y})$ . Equivalently

- (i)  $f(\mathbf{y}) \ge f(\mathbf{x}) + (\mathbf{y} \mathbf{x}) \cdot \nabla f(\mathbf{x})$  for all  $\mathbf{x}, \mathbf{y} \in S$
- (ii)  $(\mathbf{y} \mathbf{x}) \cdot (\nabla f(\mathbf{y}) \nabla f(\mathbf{x})) \ge 0$  for all  $\mathbf{x}, \mathbf{y} \in S$
- (iii) The Hessian has all  $\lambda \ge 0$  throughout the domain

The Legendre transform  $f^*$  is given by  $f^*(\mathbf{p}) = \sup_{\mathbf{x}} [\mathbf{p}.\mathbf{x} - f(\mathbf{x})]$ . The function  $f^*$  is always convex, and  $f^{**} = f$  if f is convex.

## 4 Formalisms of Dynamics (Lagrangian, Hamiltonian, and Noether)

Given the kinetic energy  $T(\mathbf{q}, \dot{\mathbf{q}}, t)$  and the potential energy  $V(\mathbf{q}, \dot{\mathbf{q}}, t)$ , the **Lagrangian** is  $L(\mathbf{q}, \dot{\mathbf{q}}, t) = T - V$ . The dynamics are given by minimising the action  $\int L dt$ .

A special case of **Noether's theorem** gives that if  $\mathbf{X}(t,s)$  is a symmetry of  $\mathbf{x}$  for some f, then  $\frac{\partial f}{\partial \dot{x}_i} \frac{dX_i}{ds}\Big|_{s=0}$  is constant (with summation convention).

The **Hamiltonian** is given by taking the Legendre transform of the Lagrangian with respect to  $\dot{\mathbf{q}}$  (generalised velocity) to introduce  $\mathbf{p}$ , the generalised momentum. Assuming convexity of L with respect to  $\dot{\mathbf{q}}$ , the Hamiltonian can be expressed as  $H(\mathbf{q}, \mathbf{p}, t) = \mathbf{p}.\dot{\mathbf{q}} - L(\mathbf{q}, \dot{\mathbf{q}}, t)$  with  $\dot{\mathbf{q}}$  such that  $\mathbf{p} = \frac{dL}{d\dot{\mathbf{q}}}$ . The consequence of minimising action of is **Hamilton's equations**:

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

If the system does not depend explicitly on time, H is constant.