Multidim minimization (very similar)

Consider scalar function ϕ of many coords

$x_0, x_1, \ldots x_{n-1} \Rightarrow \phi(\vec{x})$

Taylor expand about small step $\vec{x} + \vec{q}$

$$\phi(\vec{x} + \vec{q}) = \phi(\vec{x}) + (\nabla\phi(\vec{x}))^T \vec{q} + \frac{1}{2}\vec{q}^{\,T} H(\vec{x})\vec{q} + O(q^3)$$

$$\nabla\phi(\vec{x}) \equiv \text{gradient vector} = \left[\frac{\partial\phi}{\partial x_0} \; \frac{\partial\phi}{\partial x_1} \; \ldots \; \frac{\partial\phi}{\partial x_{n-1}}\right]^T$$

or $(\nabla\phi(\vec{x}))^T\vec{q} = \sum \frac{\partial\phi}{\partial x_i} q_i$

To first order in slightly diff notation

$$\phi(\vec{x} + d\vec{x}) = \phi(\vec{x}) + \underbrace{\nabla\phi \cdot d\vec{x}}$$

maximum when $d\vec{x}$ points along $\nabla\phi(\vec{x})$

If local minima is $\vec{x}^*$

$$\phi(\vec{x}^* + \vec{q}) \approx \phi(\vec{x}^*) + (\nabla\phi(\vec{x}^*))^T\vec{q}$$

largest decrease when $\vec{q}$ points opposite $\nabla\phi(\vec{x}^*)$

but we are at minima so we can't get lower

$\Rightarrow \nabla\phi(\vec{x}^*) = 0$ multidimensional critical point

$\nabla \phi(\vec{x}) = 0 = \vec{f}(\vec{x})$ Same problem we already solved

recall old solution $\bar{\bar{J}}(\vec{x}^{(k-1)})(\vec{x}^{(k)} - \vec{x}^{(k-1)}) = -\vec{f}(\vec{x})^{(k-1)}$

$\Rightarrow \quad J_{\nabla\phi}(\vec{x}^{(k-1)}) * (\vec{x}^{(k)} - \vec{x}^{(k-1)}) = -\nabla\phi(\vec{x})^{(k-1)}$

where $J_{\nabla\phi}(\vec{x}) = H(\vec{x}) \equiv$ Hessian

$$H(\vec{x}) = \left\{ \frac{\partial \phi}{\partial x_i \partial x_j} \right\} = \begin{bmatrix} \frac{\partial^2 \phi}{\partial x_0^2} & \cdots\cdots & \frac{\partial^2 \phi}{\partial x_0 \partial x_{n-1}} \\ \vdots & & \\ \frac{\partial^2 \phi}{\partial x_{n-1} \partial x_0} & \cdots\cdots & \frac{\partial^2 \phi}{\partial x_{n-1}^2} \end{bmatrix}$$

<u>Action</u>

Single particle in one-dim (x)

$KE = \frac{1}{2} m \dot{x}^2 \qquad \dot{x} = dx/dt = v$

$V = V(x(t))$ potential

Lagrangian $\mathcal{L}(x(t), \dot{x}(t)) = KE(\dot{x}(t)) - V(x(t))$

We study particle from $t = 0$ to $t = \mathcal{T}$ and define the action functional

$$S[x(t)] = \int_0^{\mathcal{T}} dt \, \mathcal{L}(x(t), \dot{x}(t))$$

S is a functional $\Rightarrow$ function of a function

$f(x) \longrightarrow S \longrightarrow \#$ depends on all values of x but not of t

For given trajectory $x(t)$ from $t=0$ to $t=T$

$S[x(t)]$ gives a single number

Hamilton's principle: particle follows a trajectory that minimizes the action

(Similar to Fermat's principle for path of least time for light)

Algorithm: Discretize time $t_k = k \frac{T}{n-1} = k h_t$

where $k = 0, 1, \dots n-1$ Let $x_k = x(t_k)$

We will compute an integral by a rectangle approx and use forward diff. for $\dot{x}$

$$S_n = \sum_{k=0}^{n-2} \underbrace{h_t}_{\text{rect width}} \underbrace{\left[\frac{1}{2} m \left(\frac{x_{k+1} - x_k}{h_t} \right)^2 - V(x_k) \right]}_{\text{rect height}}$$

we keep $x(0)$ and $x(T)$ fixed by definition

$S_n = S_n(x_1, x_2, \dots x_{n-2}) \leftarrow$ need its minimum like $\phi(\vec{x})$ problem

Solution

$$J_{\nabla\phi}(\vec{x}^{(k-1)})(\vec{x}^{(k)} - \vec{x}^{(k-1)}) = -\nabla\phi(\vec{x}^{(k-1)})$$

where we use S instead of ϕ

$$\nabla S_i = \frac{\partial S_n}{\partial x_i} = \sum_{k=0}^{n-2} h_t \left[\frac{m}{h_t^2} (x_{k+1} - x_k)(\delta_{i,k+1} - \delta_{i,k}) - \frac{\partial V(x_k)}{\partial x_i} \delta_{i,k} \right]$$

$$= \frac{m}{h_t}(2x_i - x_{i-1} - x_{i+1}) - h_t \frac{\partial V(x_i)}{\partial x_i}$$

also need $J_{\nabla S}$ $\Rightarrow$ take another derivative

(Eqn 5.137)