Geodesic Equation & Hamiltonian Dynamics

Hang Shao

Introduction

- Recall Lagrangian Mechanics
- Geodesic Equations
- Hamiltonian Mechanics (Dynamics)
- Applications

Lagrangian Mechanics

- Lagrangian : $L(q^i, \dot{q}^i, t)$ short for $L(q^1, \cdots, q^n, \dot{q}^1, \cdots, \dot{q}^n, t)$

  where $\dot{q}^i = dq^i/dt$

- kinetic minus the potential energy

Lagrangian Mechanics

- Variation of Lagrangian $\delta L = \sum_{i=1}^{N}(\frac{\partial L}{\partial q_i}\delta q_i + \frac{\partial L}{\partial \dot{q}_i}\delta \dot{q}_i)$, which is similar with total differential of $L(q^i, \dot{q}^i, t)$
- Then integrate the variation with respect to time and make it to 0, which can be summarized by Hamilton's principle

$$\int_a^b \delta L = 0$$

Lagrangian Mechanics

- Integrating $\int_a^b \delta L$ by parts and boundary condition
- Euler–Lagrange equation

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}^i} - \frac{\partial L}{\partial q^i} = 0$$

Deriving Geodesic Equation via Action

- Euler-Lagrange equation :

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0$$

- Lagrangian :

$$L = \frac{1}{2}\sum_i \sum_j g_{ij}(q)\dot{q}_i \dot{q}_j$$

$$\frac{\partial L}{\partial q_j} = \frac{1}{2}\sum_i \sum_k \frac{\partial g_{ik}}{\partial q_j}\dot{q}_i \dot{q}_k$$

$$\frac{\partial L}{\partial \dot{q}_j} = \sum_k g_{jk}\dot{q}_k$$

Deriving Geodesic Equation via Action

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_j} = \frac{d}{dt}(\sum_k g_{jk}\dot{q}_k)$$

$$= \sum_k(\sum_m \frac{\partial g_{jk}}{\partial q_m}\dot{q_m}\dot{q_k} + g_{jk}\ddot{q_k})$$

$$= \frac{1}{2}\sum_k\sum_m \frac{\partial g_{jk}}{\partial q_m}\dot{q_m}\dot{q_k} + \frac{1}{2}\sum_k\sum_m \frac{\partial g_{jk}}{\partial q_m}\dot{q_m}\dot{q_k} + \sum_k g_{jk}\ddot{q_k}$$

Deriving Geodesic Equation via Action

- Combine two parts of Euler-Lagrange equation together :

$$\frac{1}{2}\sum_k\sum_m \frac{\partial g_{jk}}{\partial q_m}\dot{q_m}\dot{q_k} + \frac{1}{2}\sum_k\sum_m \frac{\partial g_{jk}}{\partial q_m}\dot{q_m}\dot{q_k} + \sum_k g_{jk}\ddot{q_k} - \frac{1}{2}\sum_k\sum_m \frac{\partial g_{km}}{\partial q_j}\dot{q_m}\dot{q_k} = 0$$

- Time g^{ij} for both sides and do summation respect index of j for above equation :

$$\frac{1}{2}\sum_j g^{ij}\sum_k\sum_m \frac{\partial g_{jk}}{\partial q_m}\dot{q}_m\dot{q}_k + \frac{1}{2}\sum_j g^{ij}\sum_k\sum_m \frac{\partial g_{jk}}{\partial q_m}\dot{q}_m\dot{q}_k + \sum_j\sum_k g_{jk}\ddot{q}_k - \frac{1}{2}\sum_j g^{ij}\sum_k\sum_m \frac{\partial g_{km}}{\partial q_j}\dot{q}_m\dot{q}_k = 0$$

Deriving Geodesic Equation via Action

- Exchange indices of m and j for the whole equation :

$$\frac{1}{2}\sum_j\sum_k\sum_m g^{im}\frac{\partial g_{mk}}{\partial q_j}\dot{q}_j\dot{q}_k + \frac{1}{2}\sum_j\sum_k\sum_m g^{im}\frac{\partial g_{mk}}{\partial q_j}\dot{q}_j\dot{q}_k - \frac{1}{2}\sum_j\sum_k\sum_m g^{im}\frac{\partial g_{jk}}{\partial q_m}\dot{q}_j\dot{q}_k + \ddot{q}_i = 0$$

- Exchange indices of j and k for the first term of equation :

$$\frac{1}{2}\sum_j\sum_k\sum_m g^{im}\frac{\partial g_{mk}}{\partial q_j}\dot{q}_j\dot{q}_k \rightarrow \frac{1}{2}\sum_k\sum_j\sum_m g^{im}\frac{\partial g_{mj}}{\partial q_k}\dot{q}_k\dot{q}_j$$

Deriving Geodesic Equation via Action

- Rearrange all terms in the equation :

$$\ddot{q}_i + \frac{1}{2}\sum_k \sum_m \sum_j g^{im}\left(\frac{\partial g_{jm}}{\partial q_k}\dot{q}_j\dot{q}_k + \frac{\partial g_{km}}{\partial q_j}\dot{q}_j\dot{q}_k - \frac{\partial g_{jk}}{\partial q_m}\dot{q}_j\dot{q}_k\right) = 0$$

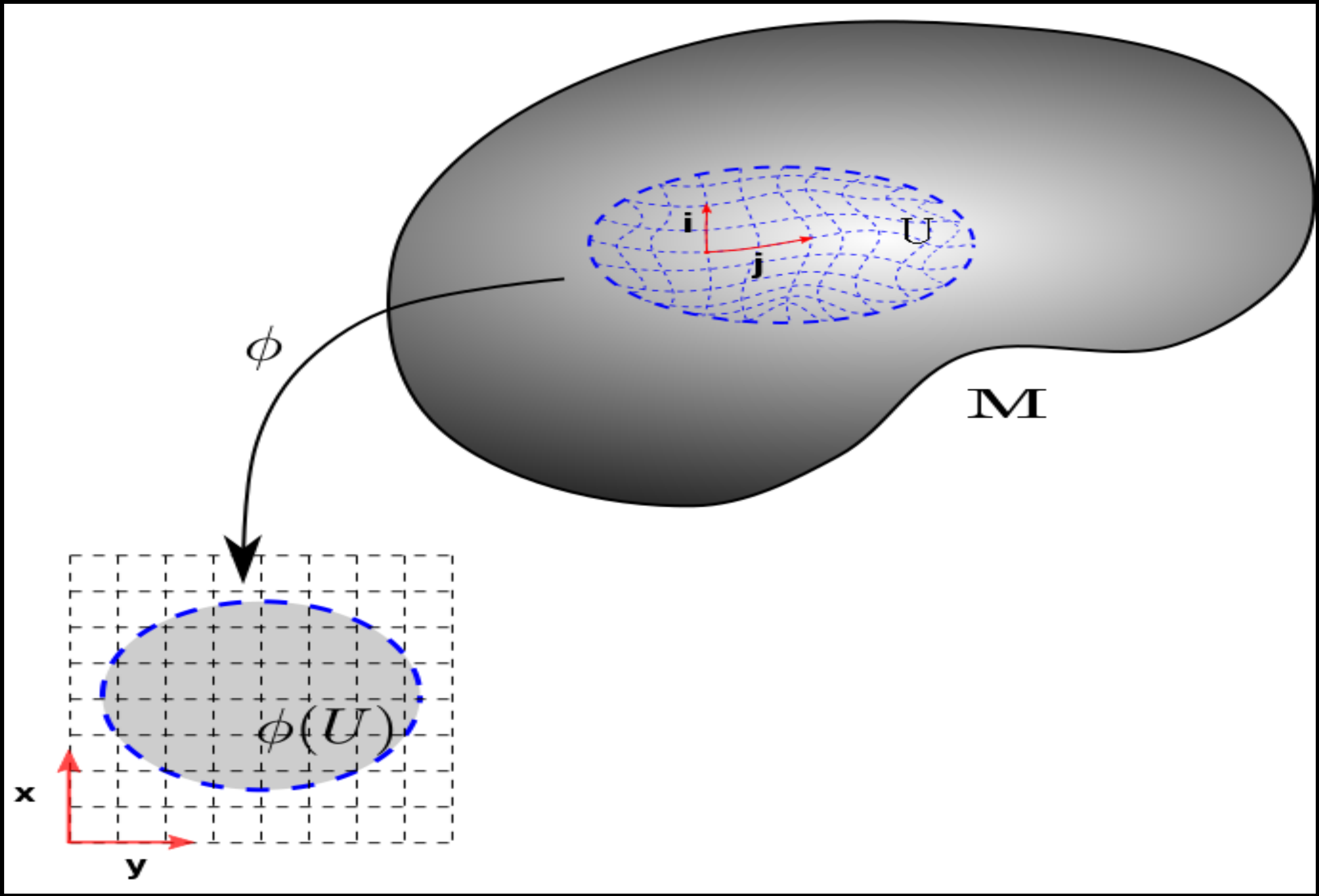
Deriving Geodesic Equation via Action

- Geodesic equation :

$$\ddot{q}_i + \sum_k \sum_j \Gamma^i_{jk} \dot{q}_j \dot{q}_k = 0$$

where $$\Gamma^i_{jk} = \frac{1}{2} \sum_m g^{im} \left(\frac{\partial g_{jm}}{\partial q_k} + \frac{\partial g_{km}}{\partial q_j} - \frac{\partial g_{jk}}{\partial q_m} \right)$$

Geodesic Equation



Geodesic Equation

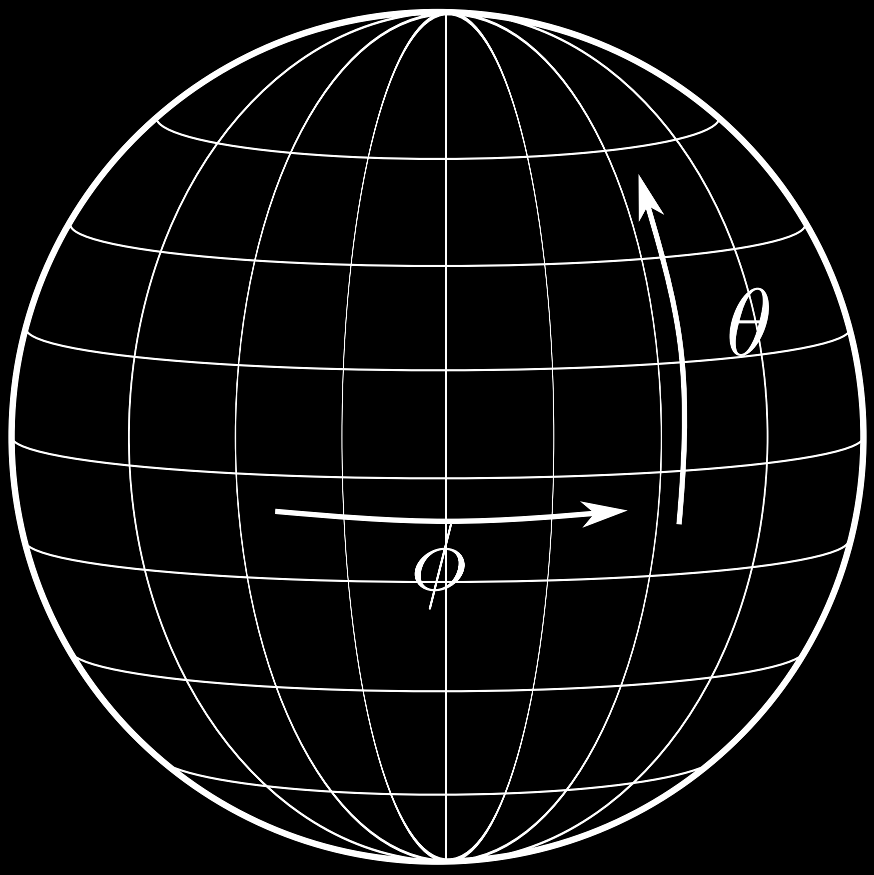
- SO(3) (S^2) coordinate chart :

$$(\cos\theta\cos\phi, \sin\theta\cos\phi, \sin\phi)$$

- Unit tangent vectors:

$$e_\theta = (-\sin\theta\cos\phi, \cos\theta\cos\phi, 0)$$
$$e_\phi = (-\cos\theta\sin\phi, -\sin\theta\sin\phi, \cos\phi)$$

$$g = \begin{pmatrix} \langle e_\theta, e_\theta \rangle & \langle e_\theta, e_\phi \rangle \\ \langle e_\phi, e_\theta \rangle & \langle e_\phi, e_\phi \rangle \end{pmatrix}$$
$$= \begin{pmatrix} (\cos\phi)^2 & 0 \\ 0 & 1 \end{pmatrix}$$



Geodesic Equation

- Differential of metric :

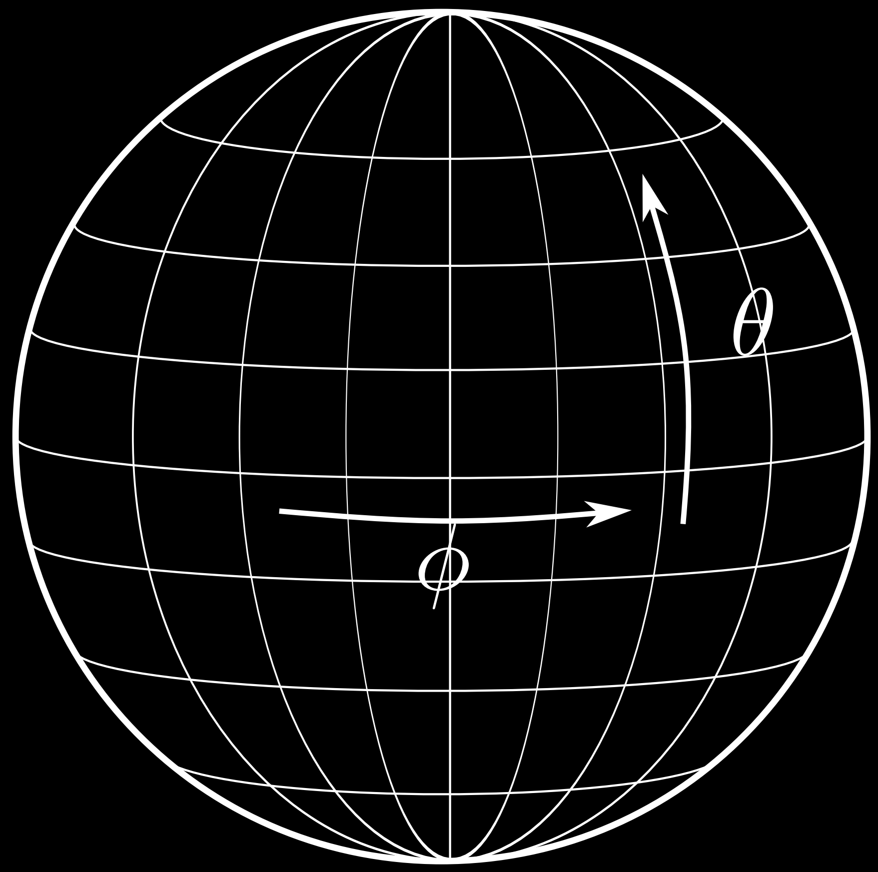
$$\frac{\partial g_{\theta\theta}}{\partial \phi} = -2\sin\phi$$

- Quaternions :

$$q(t) = (\theta(t), \phi(t))$$

$$\theta(t) = t$$

$$\phi(t) = 0$$



$$\ddot{q}(t) = 0$$

Hamiltonian Mechanics

- Conjugate momenta : $p^i = \frac{\partial L}{\partial \dot{q}^i} \qquad (q^i, \dot{q}^i) \mapsto (q^i, p_i)$

- Total differential of Lagrangian :

$$
\begin{aligned}
dL &= \sum_{i=1}^{N} \frac{\partial L}{\partial q_i} dq_i + \sum_{i=1}^{N} \frac{\partial L}{\partial \dot{q}_i} d\dot{q}_i \\
&= \sum_{i=1}^{N} \dot{p}_i dq_i + \sum_{i=1}^{N} p_i d\dot{q}_i
\end{aligned}
$$

Hamiltonian Mechanics

- Set velocities to momenta via a Legendre transformation

$$dL = \sum_{i=1}^{N} \dot{p}_i dq_i + d(p \cdot \dot{q}) - \sum_{i=1}^{N} \dot{q}_i dp_i$$

$$d(p \cdot \dot{q} - L) = -\sum_{i=1}^{N} \dot{p}_i dq_i + \sum_{i=1}^{N} \dot{q}_i dp_i$$

- Define "Hamiltonian" as

$$H = p \cdot \dot{q} - L$$

$$dH = -\sum_{i=1}^{N} \dot{p}_i dq_i + \sum_{i=1}^{N} \dot{q}_i dp_i$$

Hamiltonian Mechanics

- Hamiltonian equations :

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

Hamiltonian Mechanics

- Assumed kinetic energy is $T =< \dot{q}, \dot{q} >= \sum_{i,j=1}^{N} c_{ij} \dot{q}_i \dot{q}_j$

$$\frac{\partial T}{\partial \dot{q}_j} = 2 \sum_{i=1}^{N} c_{ij} \dot{q}_i$$

$$\begin{aligned} H &= \sum_{i=1}^{N} \dot{p}_i \frac{\partial L}{\partial \dot{q}_i} - L \\ &= \sum_{i=1}^{N} \dot{p}_i \frac{\partial T}{\partial \dot{q}_i} - L \\ &= 2T - L \\ &= T + U \end{aligned}$$

Geodesic Equations

- Lagrangian and Hamiltonian

$$L = \frac{1}{2}\sum_i \sum_j g_{ij}(q)\dot{q}_i \dot{q}_j$$

$$H = \frac{1}{2}\sum_i \sum_j g^{ij}(q) p_i p_j$$

- Metrics and inverse of it

$$g^{ij} g_{jk} = \delta^i_k$$

- Hamiltonian Equation

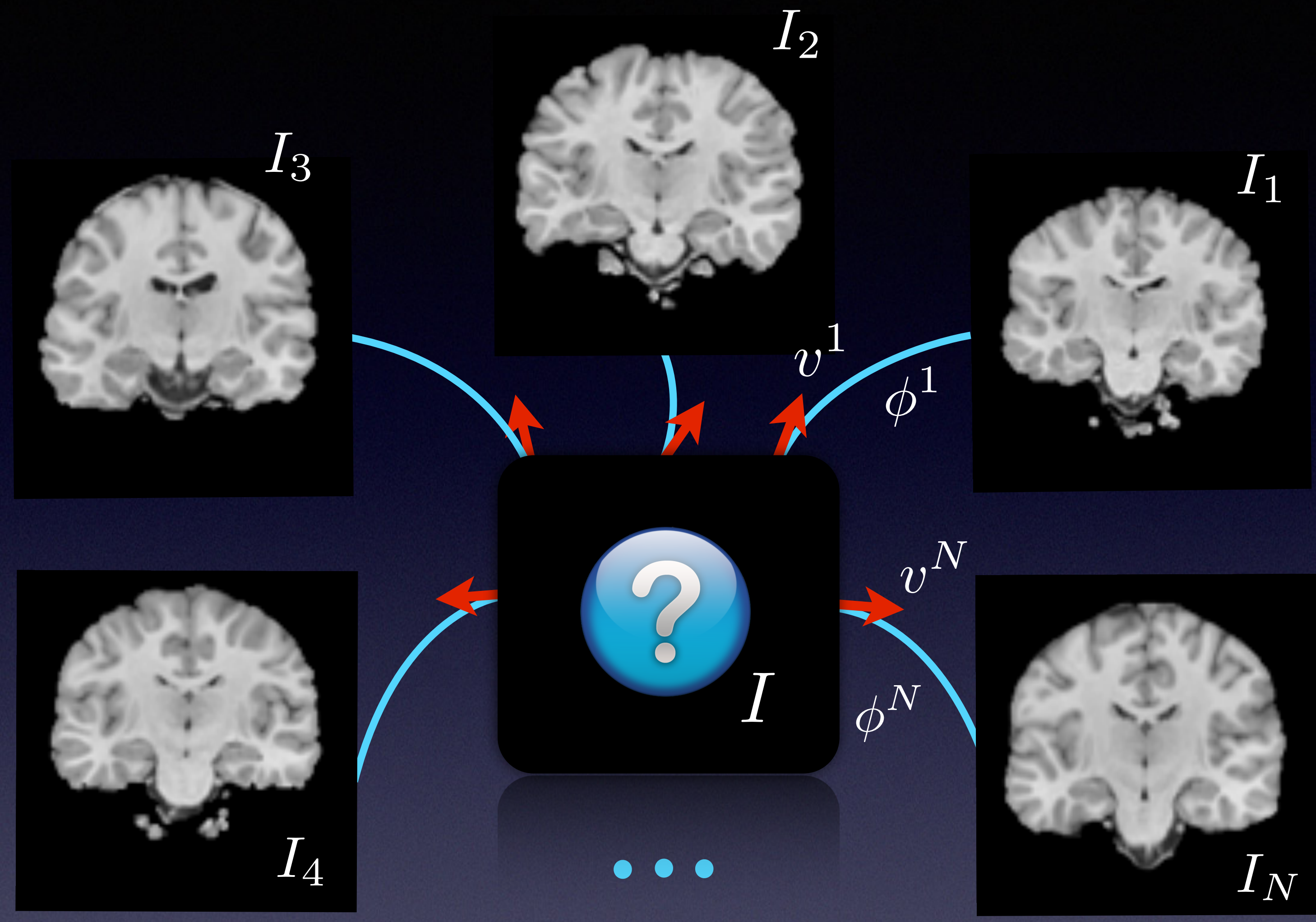
$$\frac{dq_i}{dt} = g^{ij} p_i$$

$$\frac{dp_i}{dt} = -\frac{1}{2}\frac{\partial g^{jk}}{\partial q_i} p_j p_k$$

Applications of Hamiltonian

- Geodesic Flow
- Image Registration
- Hamiltonian Monte Carlo Sampling(HMC Sampling)

Single Atlas Estimation



$$E(I, v^k) = \sum_{k=1}^{N} \frac{1}{2\sigma^2} \|I \circ (\phi^k)^{-1} - I_k\|^2 + (Lv^k, v^k)$$

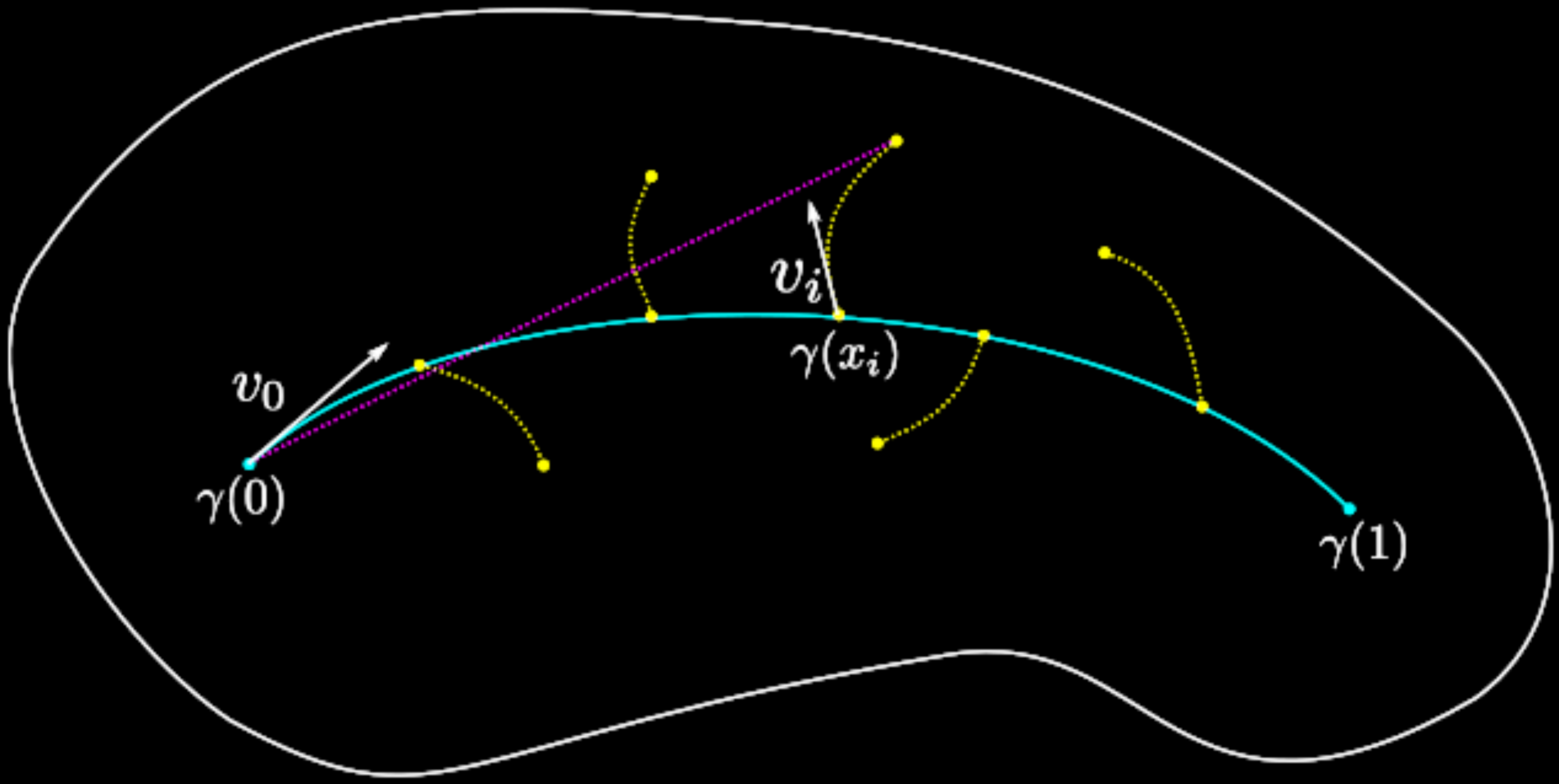
Laplacian operator: $L = -\alpha\Delta + \epsilon$

$\alpha > 0$: regularization parameter

σ^2: noise variance

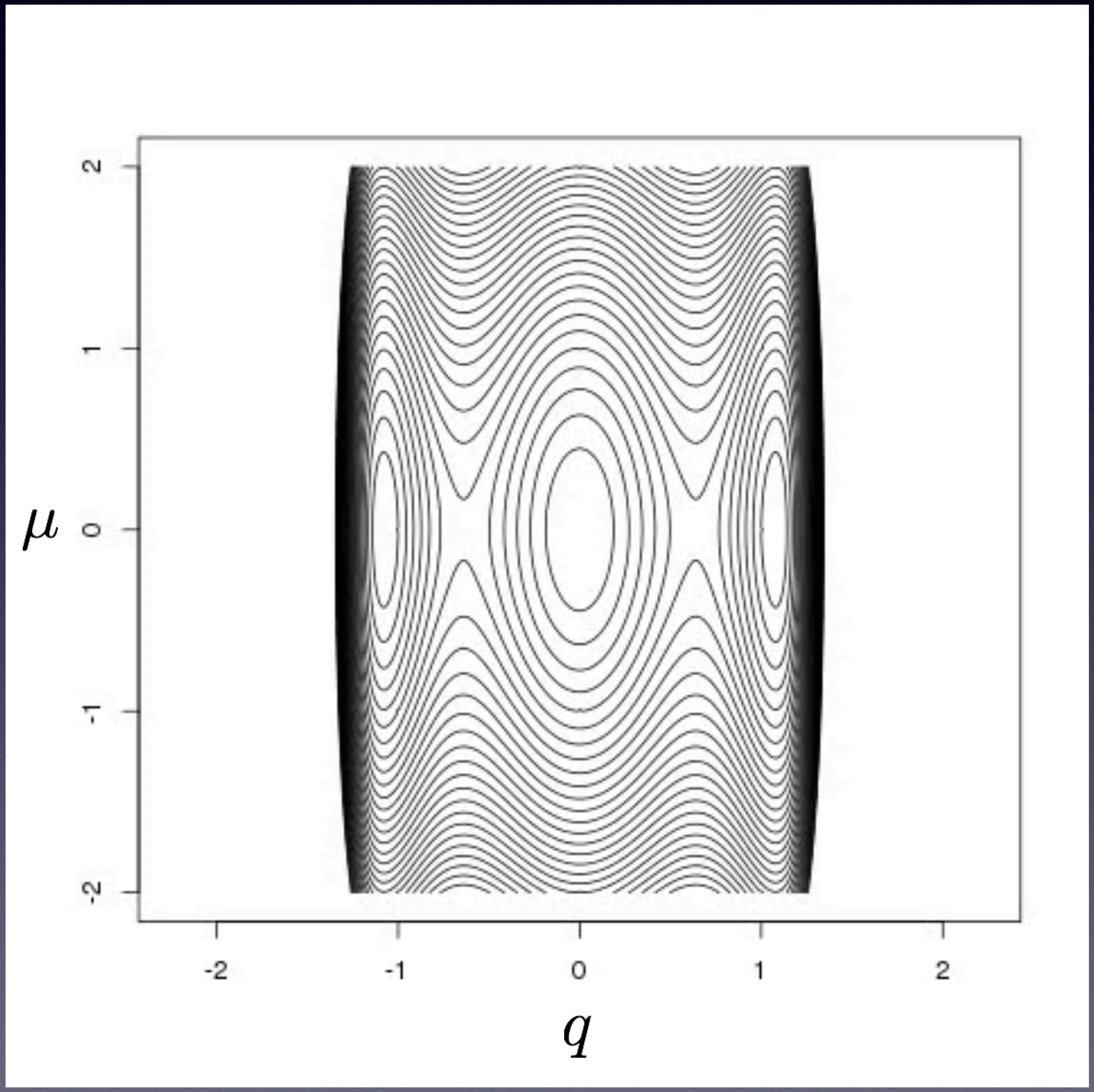
Vialard et al. 2011

Geodesic Regression



HMC Sampling

HMC efficiently explores the distribution space with high acceptance rates.



Hamiltonian Dynamics:

$$H(q, \mu) = U(q) + T(\mu)$$

- sample q, $P(q) \propto \exp\left(-U(q)\right)$
- random auxiliary variable μ, i.i.d. Gaussian

Acceptance-rejection method:

$$P(\text{accept}) = \min\left(1,\ \exp(-H(\tilde{q}, \tilde{\mu}) + H(q, \mu))\right)$$