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
  \[ \delta L = \sum_{i=1}^{N} \left( \frac{\partial L}{\partial q_i} \delta q_i + \frac{\partial L}{\partial \dot{q}_i} \delta \dot{q}_i \right) \]

  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

\[
\frac{d}{dt} \frac{\partial L}{\partial \dot{q}_j} = \frac{d}{dt} \left( \sum_k g_{jk} \dot{q}_k \right)
\]

\[
= \sum_k \left( \sum_m \frac{\partial g_{jk}}{\partial q_m} q_m \dot{q}_k + g_{jk} \ddot{q}_k \right)
\]

\[
= \frac{1}{2} \sum_k \sum_m \frac{\partial g_{jk}}{\partial q_m} q_m \dot{q}_k + \frac{1}{2} \sum_k \sum_m \frac{\partial g_{jk}}{\partial q_m} q_m q_k + \sum_k g_{jk} \ddot{q}_k
\]
Deriving Geodesic Equation via Action

• Combine two parts of Euler-Lagrange equation together:

\[
\frac{1}{2} \sum_k \sum_m \frac{\partial g_{jk}}{\partial q_m} \dot{q}_m \dot{q}_k + \frac{1}{2} \sum_k \sum_m \frac{\partial g_{jk}}{\partial q_m} \dot{q}_m \dot{q}_k + \sum_k g_{jk} \ddot{q}_k - \frac{1}{2} \sum_k \sum_m \frac{\partial g_{jm}}{\partial q_j} q_m q_k = 0
\]

• Time \( g^{ij} \) for both sides and do summation respect index of j for above equation:

\[
\frac{1}{2} \sum_j g^{ij} \sum_k \sum_m \frac{\partial g_{jk}}{\partial q_m} \dot{q}_m \dot{q}_k + \frac{1}{2} \sum_j g^{ij} \sum_k \sum_m \frac{\partial g_{jk}}{\partial q_m} \dot{q}_m \dot{q}_k + \sum_j \sum_k g_{jk} \ddot{q}_k - \frac{1}{2} \sum_j g^{ij} \sum_k \sum_m \frac{\partial g_{jm}}{\partial q_j} q_m q_k = 0
\]
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:

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

• Geodesic equation:

\[ \ddot{q}_i + \sum_{k} \sum_{j} \Gamma_{jk}^{i} \dot{q}_j \dot{q}_k = 0 \]

where

\[ \Gamma_{jk}^{i} = \frac{1}{2} \sum_{m} g^{im} \left( \frac{\partial g_{jm}}{\partial q_{k}} + \frac{\partial g_{km}}{\partial q_{j}} - \frac{\partial g_{jk}}{\partial q_{m}} \right) \]
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: \( p^i = \frac{\partial L}{\partial \dot{q}^i} \) \( (q^i, \dot{q}^i) \mapsto (q^i, p_i) \)

- Total differential of Lagrangian:

\[
dL = \sum_{i=1}^N \frac{\partial L}{\partial q_i} dq_i + \sum_{i=1}^N \frac{\partial L}{\partial \dot{q}_i} d\dot{q}_i
\]

\[
= \sum_{i=1}^N \dot{p}_i dq_i + \sum_{i=1}^N p_i d\dot{q}_i
\]
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 \( T = \langle \dot{q}, \dot{q} \rangle = \sum_{i,j=1}^{N} c_{ij} \dot{q}_i \dot{q}_j \)

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

\[
H = \sum_{i=1}^{N} \dot{p}_i \frac{\partial L}{\partial \dot{q}_i} - L
\]

\[
= \sum_{i=1}^{N} \dot{p}_i \frac{\partial T}{\partial \dot{q}_i} - L
\]

\[
= 2T - L
\]

\[
= T + U
\]
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

\[ \frac{dq_i}{dt} = g^{ij} p_j \]
\[ \frac{dp_i}{dt} = -\frac{1}{2} \frac{\partial g^{jk}}{\partial q_i} p_j p_k \]
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
\( \sigma^2 \): 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 \( q \), \( P(q) \propto \exp(-U(q)) \)
- random auxiliary variable \( \mu \), i.i.d. Gaussian

Acceptance-rejection method:

\[ P(\text{accept}) = \min(1, \exp(-H(\tilde{q}, \tilde{\mu}) + H(q, \mu))) \]