CSE 291 (SP25)
Physics Simulation
Calculus of Variations

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What is calculus of variations?

- In **calculus**, we take derivatives of **functions of a few variables**.
- In **calculus of variations**, we take derivatives of **functions of functions** (also known as **functionals**).
- Main purpose: formulate optimization problem over function spaces and derive its optimality condition (KKT condition)
- These optimality conditions are often differential equations (called **Euler–Lagrange equations**)
- Most physical equations arise as the Euler–Lagrange equation.
- Allow replacing “modeling forces” to “designing one functional.”

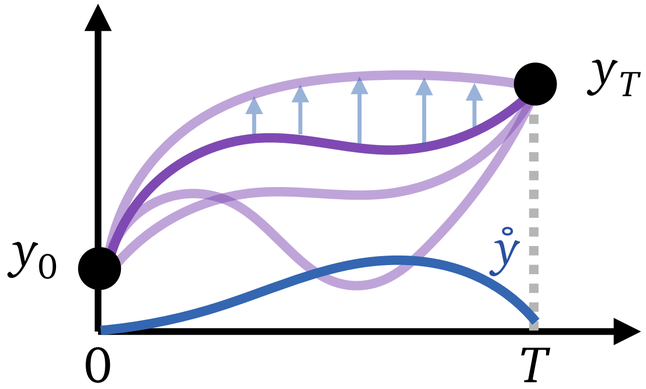
First Example

- Example 1
- General Euler–Lagrange equation
- Least action principle
- Example 2: Compound pendulum
- Noether’s theorem of time independence
- Example 3: Hanging chain
- Example 4: Mass spring system

Example1

- Let $\mathcal{M} = \{y : [0, T] \to \mathbb{R} \mid y(0) = y_0, y(T) = y_T\}$
- $\mathcal{E} : \mathcal{M} \to \mathbb{R}$

$$\mathcal{E}(y) := \int_{t=0}^{T} \left(\frac{1}{2} y'(t)^2 + \cos(y(t)) \right) dt$$



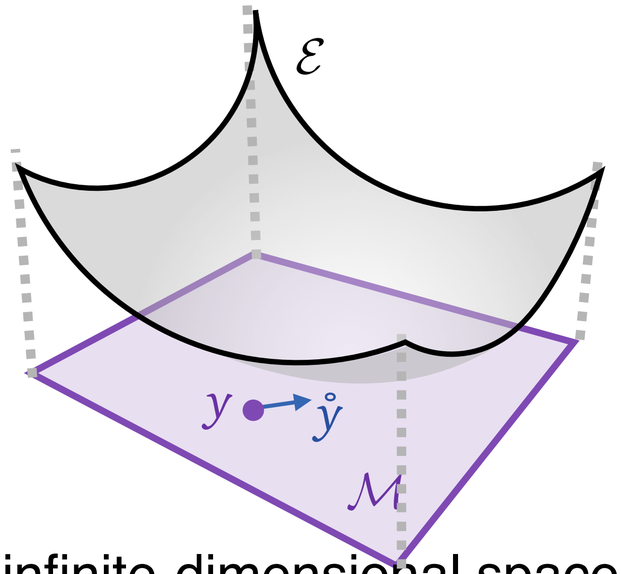
Problem

What is the optimality condition for

$$\underset{y \in \mathcal{M}}{\text{minimize}}\ \mathcal{E}(y)$$

- The optimality is

$$d\mathcal{E}_y[\![\mathring{y}]\!] = 0 \quad \forall\, \mathring{y} \in T_y\mathcal{M}$$

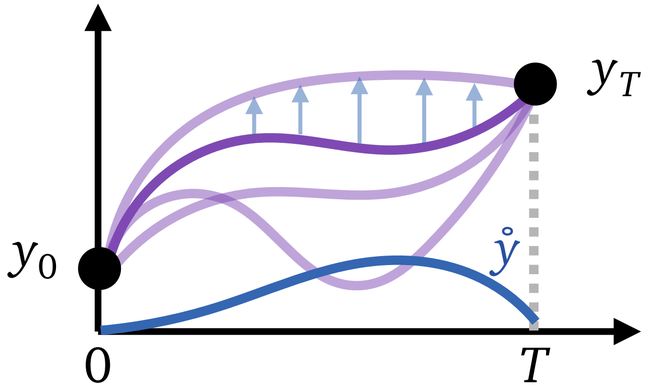


infinite-dimensional space

Example1

- Let $\mathcal{M} = \{y : [0, T] \to \mathbb{R} \mid y(0) = y_0, y(T) = y_T\}$
- $\mathcal{E} : \mathcal{M} \to \mathbb{R}$

$$\mathcal{E}(y) := \int_{t=0}^{T} \left(\frac{1}{2} y'(t)^2 + \cos(y(t)) \right) dt$$



- The optimality is

$$d\mathcal{E}_y[\![\mathring{y}]\!] = 0 \quad \forall\, \mathring{y} \in T_y\mathcal{M} = \{\mathring{y} : [0, T] \to \mathbb{R} \mid \mathring{y}(0) = \mathring{y}(T) = 0\}$$

$$0 = d\mathcal{E}_y[\![\mathring{y}]\!] = \frac{d}{d\epsilon}\Big|_{\epsilon=0} \mathcal{E}(y + \epsilon\mathring{y})$$

$$= \frac{d}{d\epsilon}\Big|_{\epsilon=0} \int_{t=0}^{T} \left(\frac{1}{2}(y' + \epsilon\mathring{y}')^2 + \cos(y + \epsilon\mathring{y}) \right) dt$$

$$= \int_{t=0}^{T} (y'\mathring{y}' - \sin(y)\mathring{y})\, dt$$

Example1

$$\forall\, \mathring{y} \in T_y\mathcal{M} = \{\mathring{y} : [0,T] \to \mathbb{R} \,|\, \mathring{y}(0) = \mathring{y}(T) = 0\}$$

$$\begin{aligned}
0 = d\mathcal{E}_y[\![\mathring{y}]\!] &= \frac{d}{d\epsilon}\Big|_{\epsilon=0} \mathcal{E}(y + \epsilon\mathring{y}) \\
&= \frac{d}{d\epsilon}\Big|_{\epsilon=0} \int_{t=0}^{T} \left(\tfrac{1}{2}(y' + \epsilon\mathring{y}')^2 + \cos(y + \epsilon\mathring{y})\right) dt \\
&= \int_{t=0}^{T} (y'\mathring{y}' - \sin(y)\mathring{y})\, dt \\
&= \int_{t=0}^{T} (-y''\mathring{y} - \sin(y)\mathring{y})\, dt \\
&= -\int_{t=0}^{T} (y'' + \sin(y))\,\mathring{y}\, dt
\end{aligned}$$

$$\Longrightarrow \quad \boxed{y''(t) + \sin(y(t)) = 0} \qquad \textbf{pendulum equation}$$

Example1

- $\mathcal{E} : \mathcal{M} \to \mathbb{R}$

  $\mathcal{E}(y) := \int_{t=0}^{T} \left(\frac{1}{2} y'(t)^2 + \cos(y(t)) \right) dt$

variational formulation for the pendulum system

Problem

What is the optimality condition for

$$\underset{y \in \mathcal{M}}{\text{minimize}}\ \mathcal{E}(y)$$

$$\Longrightarrow \quad \boxed{y''(t) + \sin(y(t)) = 0}$$

pendulum equation

General Euler–Lagrange Equation

- Example 1
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A common form of variational problem

- $\mathcal{M} = \{\mathbf{y} : [0, T] \to \mathbb{R}^m \mid \mathbf{y}(0) = \mathbf{y}_0, \mathbf{y}(T) = \mathbf{y}_T\}$
- $T_{\mathbf{y}}\mathcal{M} = \{\mathring{\mathbf{y}} : [0, T] \to \mathbb{R}^m \mid \mathring{\mathbf{y}}(0) = \mathring{\mathbf{y}}(T) = \mathbf{0}\}$
- $\mathcal{E}(\mathbf{y}) := \int_0^T L(t, \mathbf{y}(t), \mathbf{y}'(t))\, t$

  for some integrand expression $L : [0, T] \times \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R}$
- Directional derivative:

$$d\mathcal{E}_{\mathbf{y}}[\![\mathring{\mathbf{y}}]\!] = \frac{d}{d\epsilon}\Big|_{\epsilon=0} \mathcal{E}(\mathbf{y} + \epsilon\mathring{\mathbf{y}})$$

$$= \int_0^T \frac{\partial}{\partial\epsilon}\Big|_{\epsilon=0} L\big(t, \mathbf{y}(t) + \epsilon\mathring{\mathbf{y}}(t), \mathbf{y}'(t) + \epsilon\mathring{\mathbf{y}}'(t)\big)\, dt$$

A common form of variational problem

$$d\mathcal{E}_{\mathbf{y}}[\![\mathring{\mathbf{y}}]\!] = \frac{d}{d\epsilon}\Big|_{\epsilon=0}\mathcal{E}(\mathbf{y}+\epsilon\mathring{\mathbf{y}})$$

$$= \int_0^T \frac{\partial}{\partial\epsilon}\Big|_{\epsilon=0} L\big(t, \mathbf{y}(t)+\epsilon\mathring{\mathbf{y}}(t), \mathbf{y}'(t)+\epsilon\mathring{\mathbf{y}}'(t)\big)\,dt$$

$$= \int_0^T \Big\langle \frac{\partial L}{\partial \mathbf{y}}_{(t,\mathbf{y}(t),\mathbf{y}'(t))} \Big| \mathring{\mathbf{y}}(t) \Big\rangle\, dt + \int_0^T \Big\langle \frac{\partial L}{\partial \mathbf{y}'}_{(t,\mathbf{y}(t),\mathbf{y}'(t))} \Big| \mathring{\mathbf{y}}'(t) \Big\rangle\, dt$$

$$= \int_0^T \Big\langle \frac{\partial L}{\partial \mathbf{y}}_{(t,\mathbf{y}(t),\mathbf{y}'(t))} \Big| \mathring{\mathbf{y}}(t) \Big\rangle\, dt - \int_0^T \Big\langle \frac{d}{dt}\Big(\frac{\partial L}{\partial \mathbf{y}'}_{(t,\mathbf{y}(t),\mathbf{y}(t))} \Big) \Big| \mathring{\mathbf{y}}(t) \Big\rangle\, dt$$

$$= \int_0^T \Big\langle \frac{\partial L}{\partial \mathbf{y}}_{(t,\mathbf{y}(t),\mathbf{y}'(t))} - \frac{d}{dt}\Big(\frac{\partial L}{\partial \mathbf{y}'}_{(t,\mathbf{y}(t),\mathbf{y}(t))} \Big) \Big| \mathring{\mathbf{y}}(t) \Big\rangle\, dt$$

A common form of variational problem

$$\mathcal{E}(\mathbf{y}) := \int_0^T L(t, \mathbf{y}(t), \mathbf{y}'(t))\, t$$

$$d\mathcal{E}_{\mathbf{y}}[\![\mathring{\mathbf{y}}]\!] = \int_0^T \left\langle \frac{\partial L}{\partial \mathbf{y}}_{(t,\mathbf{y}(t),\mathbf{y}'(t))} - \frac{d}{dt}\left(\frac{\partial L}{\partial \mathbf{y}'}_{(t,\mathbf{y}(t),\mathbf{y}(t))} \right) \middle| \mathring{\mathbf{y}}(t) \right\rangle dt$$

- Convention notation for functional derivative:

$$\frac{\delta \mathcal{E}}{\delta \mathbf{y}}(t) = \frac{\partial L}{\partial \mathbf{y}}_{(t,\mathbf{y}(t),\mathbf{y}'(t))} - \frac{d}{dt}\left(\frac{\partial L}{\partial \mathbf{y}'}_{(t,\mathbf{y}(t),\mathbf{y}'(t))} \right)$$

- Interpret this derivative as:

$$d\mathcal{E}_{\mathbf{y}} = \int_0^T \left\langle \frac{\delta \mathcal{E}}{\delta \mathbf{y}} \middle| \cdot \right\rangle dt$$

Euler–Lagrange equation

Theorem

The optimality condition for $\underset{\mathbf{y}\in\mathcal{M}}{\text{minimize}}\ \mathcal{E}(\mathbf{y})$ with

$$\mathcal{E}(\mathbf{y}) := \int_0^T L(t, \mathbf{y}(t), \mathbf{y}'(t))\, t$$

is given by

$$\frac{\delta \mathcal{E}}{\delta \mathbf{y}}(t) = \frac{\partial L}{\partial \mathbf{y}}_{(t,\mathbf{y}(t),\mathbf{y}'(t))} - \frac{d}{dt}\left(\frac{\partial L}{\partial \mathbf{y}'}_{(t,\mathbf{y}(t),\mathbf{y}'(t))}\right) = 0$$

known as the ***Euler–Lagrange equation.***

Least Action Principle

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Many particle system

- Let $\mathbf{y}(t): [0, T] \to \mathbb{R}^{3N}$ represents position of *N* particles.
- Call $\mathbf{v}(t) := \dot{\mathbf{y}}(t)$
- Suppose the dynamics of the particles is govern by Newton's law

$$\frac{d}{dt}\mathbf{M}\mathbf{v}(t) = \mathbf{f}(\mathbf{y}(t))$$

for a mass matrix $\mathbf{M} \in \mathbb{R}^{3N \times 3N}$ and a force model $\mathbf{f}: \mathbb{R}^{3N} \to \mathbb{R}^{3N}$.

- The kinetic energy: $K(\mathbf{y}, \mathbf{v}) = \frac{1}{2}\mathbf{v}^{\mathsf{T}}\mathbf{M}\mathbf{v}$
- The potential energy: $U(\mathbf{y})$ is a function of positions $U: \mathbb{R}^{3N} \to \mathbb{R}$

so that $-\frac{\partial U}{\partial \mathbf{y}}\Big|_{\mathbf{y}} = \mathbf{f}(\mathbf{y})$ (existence of potential $\iff$ assuming force is conservative)

Many particle system

Theorem (Least action principle)

The Newton's law of motion

$$\frac{d}{dt}\mathbf{M}\mathbf{v}(t) = \mathbf{f}(\mathbf{y}(t))$$

is the Euler–Lagrange equation for the ***total action functional***

$$\mathcal{S}(\mathbf{y}) := \int_0^T L\big(\mathbf{y}(t), \dot{\mathbf{y}}(t)\big)\, dt$$

where $L(\mathbf{y}, \mathbf{v}) := K(\mathbf{y}, \mathbf{v}) - U(\mathbf{y})$ is called ***Lagrangian*** with

- The kinetic energy: $K(\mathbf{y}, \mathbf{v}) = \frac{1}{2}\mathbf{v}^\intercal \mathbf{M}\mathbf{v}$
- The potential energy: $U(\mathbf{y})$ so that $-\frac{\partial U}{\partial \mathbf{y}}\Big|_{\mathbf{y}} = \mathbf{f}(\mathbf{y})$

Many particle system

$$L(\mathbf{y}, \mathbf{v}) := K(\mathbf{y}, \mathbf{v}) - U(\mathbf{y})$$

- The kinetic energy: $K(\mathbf{y}, \mathbf{v}) = \frac{1}{2}\mathbf{v}^\intercal \mathbf{M}\mathbf{v}$
- The potential energy: $U(\mathbf{y})$ so that $-\frac{\partial U}{\partial \mathbf{y}}\Big|_{\mathbf{y}} = \mathbf{f}(\mathbf{y})$

(Proof) $$\frac{\partial L}{\partial \mathbf{y}} - \frac{d}{dt}\frac{\partial L}{\partial \mathbf{v}} = 0$$

$$\Longrightarrow \quad -\frac{\partial U}{\partial \mathbf{y}} - \frac{d}{dt}\frac{\partial K}{\partial \mathbf{v}} = 0$$

$$\Longrightarrow \quad \mathbf{f}(\mathbf{y}) - \frac{d}{dt}\mathbf{M}\mathbf{v} = 0$$

Applicability

- The least-action principle (or stationary-action principle) works for any conservative system made of particles
  - Elastic body
  - Fluids
  - Rigid body
- There are systems with non-conservative (dissipative) forces, such as viscosity, heat, friction,… least action doesn’t directly apply.

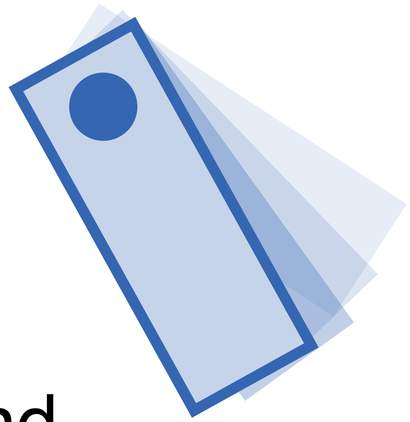
Why variational principle?

If least action principle is equivalent to Newton's *f = ma*, what is the point?

- **Reduced order modeling (generalized coordinates)**
- **Derive structure-preserving discretizations**

Why variational principle?

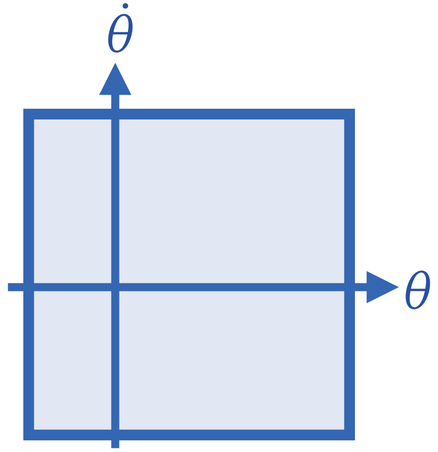
- **Reduced order modeling (generalized coordinates)**
  - A rigid object, e.g. a bar-pendulum, consists of near-infinite number of particles. Accounting all forces acting on each other is impossible.
  - It is not obvious how rigid body notions like torque and angular momentum should arise from Newton's laws.
  - Knowing that macroscopically the rigid body system can only move in a few degrees of freedom, we can parameterize the location of each particle using smaller coordinates.

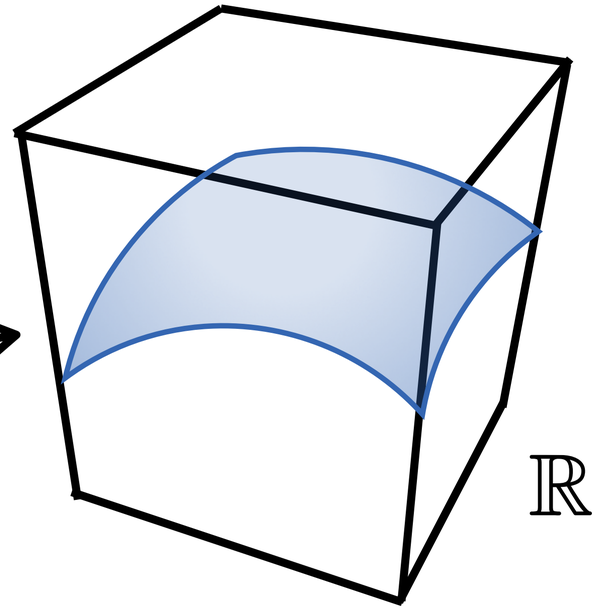


Why variational principle?

- **Reduced order modeling (generalized coordinates)**

parameter space: angle and its velocity







$\mathbb{R}^\infty$ space of positions and velocities of all particles in the body

  - It is easy to pullback the Lagrangian from particle system to the parameter space, and derive the eq of motion.

Why variational principle?

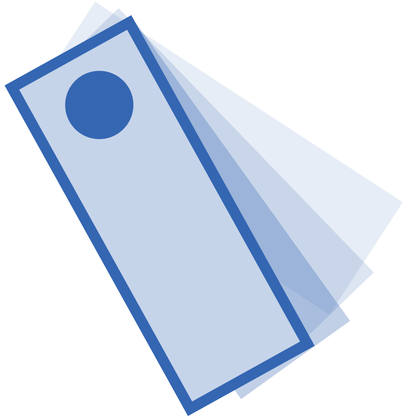
- **Reduced order modeling (generalized coordinates)**
- **Derive structure-preserving discretizations**
  - Discretize action and derive its minimization condition
  - Exact conservation of energy / momenta

Example 2: Compound Pendulum

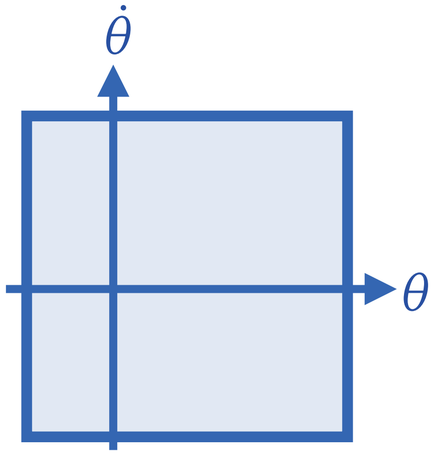
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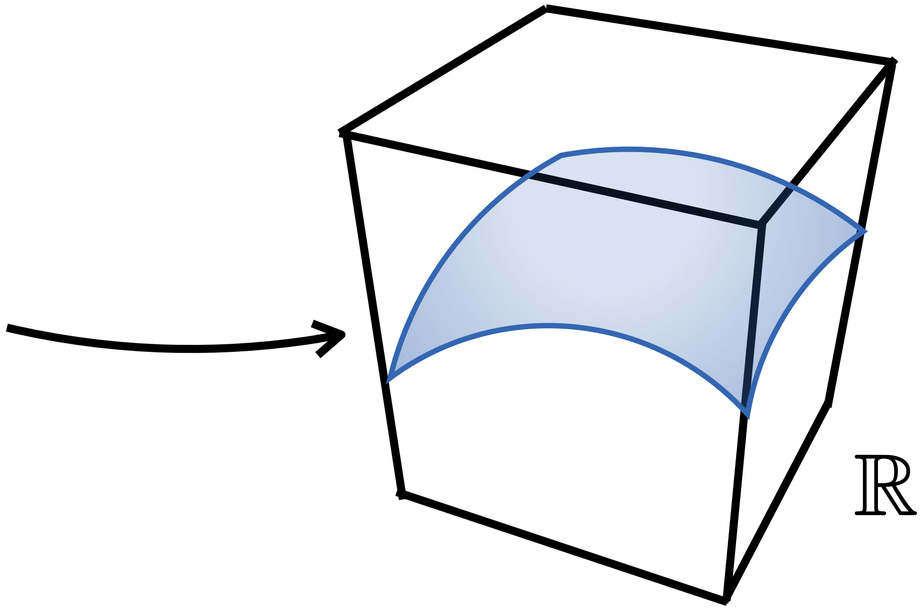
Compound pendulum

- A compound pendulum is a physically realistic pendulum, consisting a rigid body a fixed point (instead of a point mass pendulum)
- Parameterize all atoms' location by an angle variable.



parameter space: angle and its velocity

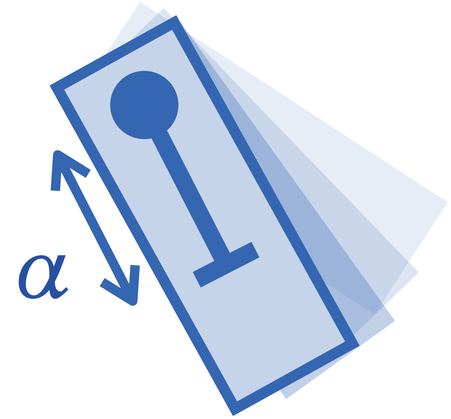




$\mathbb{R}^\infty$ space of positions and velocities of all particles in the body

Compound pendulum

- A compound pendulum is a physically realistic pendulum, consisting a rigid body a fixed point (instead of a point mass pendulum)



- Parameterize all atoms' location by an angle variable.
  - Position of α-th particle $\begin{bmatrix} x(\theta,\alpha) \\ y(\theta,\alpha) \end{bmatrix} = \begin{bmatrix} \alpha \sin\theta \\ -\alpha\cos\theta \end{bmatrix}$ $0 \le \alpha \le \ell$
  - Its velocity $\frac{d}{dt}\begin{bmatrix} x(\theta,\alpha) \\ y(\theta,\alpha) \end{bmatrix} = \begin{bmatrix} \alpha\cos\theta \\ \alpha\sin\theta \end{bmatrix}\dot{\theta}$

Compound pendulum

- Position of α-th particle $\begin{bmatrix} x(\theta,\alpha) \\ y(\theta,\alpha) \end{bmatrix} = \begin{bmatrix} \alpha\sin\theta \\ -\alpha\cos\theta \end{bmatrix} \quad 0 \le \alpha \le \ell$
- Its velocity $\dfrac{d}{dt}\begin{bmatrix} x(\theta,\alpha) \\ y(\theta,\alpha) \end{bmatrix} = \begin{bmatrix} \alpha\cos\theta \\ \alpha\sin\theta \end{bmatrix}\dot{\theta}$
- Mass of the particle $\frac{m}{\ell}d\alpha$
- Total kinetic energy $K(\theta,\dot{\theta}) = \int_0^\ell \frac{1}{2}\frac{m}{\ell}(\alpha\dot{\theta})^2 d\alpha = \frac{m\ell^2}{6}\dot{\theta}^2$
- Total potential energy $U(\theta) = \int_0^\ell \frac{mg}{\ell}(-\alpha\cos\theta)\,d\alpha$

$$= -\frac{mg\ell}{2}\cos\theta$$

Compound pendulum

- Total kinetic energy $K(\theta, \dot{\theta}) = \frac{m\ell^2}{6}\dot{\theta}^2$
- Total potential energy $U(\theta) = -\frac{mg\ell}{2}\cos\theta$

- Lagrangian $L(\theta, \dot{\theta}) = K(\theta, \dot{\theta}) - U(\theta)$
- Euler–Lagrange equation $\frac{\partial L}{\partial \theta}(\theta, \dot{\theta}) - \frac{d}{dt}\frac{\partial L}{\partial \dot{\theta}}(\theta, \dot{\theta}) = 0$

$$-\frac{mg\ell}{2}\sin\theta - \frac{m\ell^2}{3}\ddot{\theta} = 0$$

$$\boxed{\ddot{\theta} = -\frac{3}{2}\frac{g}{\ell}\sin\theta}$$

Noether’s Theorem for Time Independence

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Noether's Theorem (time independence)

Theorem

If the Lagrangian expression is time independent:

$$L(t, \mathbf{y}, \dot{\mathbf{y}}) = L(\mathbf{y}, \dot{\mathbf{y}})$$

then the Euler–Lagrange ODE $\frac{\partial L}{\partial \mathbf{y}}(\mathbf{y}, \dot{\mathbf{y}}) - \frac{d}{dt}\frac{\partial L}{\partial \dot{\mathbf{y}}}(\mathbf{y}, \dot{\mathbf{y}}) = 0$

implies that $\left\langle \frac{\partial L}{\partial \dot{\mathbf{y}}}(\mathbf{y}, \dot{\mathbf{y}}) \middle| \dot{\mathbf{y}} \right\rangle - L(\mathbf{y}, \dot{\mathbf{y}})$ is time-independent.

(Proof) Check

$$\frac{d}{dt}\left(\left\langle \frac{\partial L}{\partial \dot{\mathbf{y}}}(\mathbf{y}, \dot{\mathbf{y}}) \middle| \dot{\mathbf{y}} \right\rangle - L(\mathbf{y}, \dot{\mathbf{y}})\right) = 0$$

Noether's Theorem (time independence)

$\left\langle \frac{\partial L}{\partial \dot{\mathbf{y}}}(\mathbf{y}, \dot{\mathbf{y}}) \middle| \dot{\mathbf{y}} \right\rangle - L(\mathbf{y}, \dot{\mathbf{y}})$ is time-independent.

- For $L = \frac{1}{2}\dot{\mathbf{y}}^{\mathsf{T}}\mathbf{M}\dot{\mathbf{y}} - U(\mathbf{y})$

  this time-independent quantity is the total energy

  $$E = \frac{1}{2}\dot{\mathbf{y}}^{\mathsf{T}}\mathbf{M}\dot{\mathbf{y}} + U(\mathbf{y})$$

- Time-independence of the Lagrangian implies energy conservation.

Example 3: Shape of a Hanging Chain

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Hanging chain

- What is the shape of a hanging chain?



- It is the curve with lowest potential energy with fixed total length.

Hanging chain

- Let the shape be the function graph

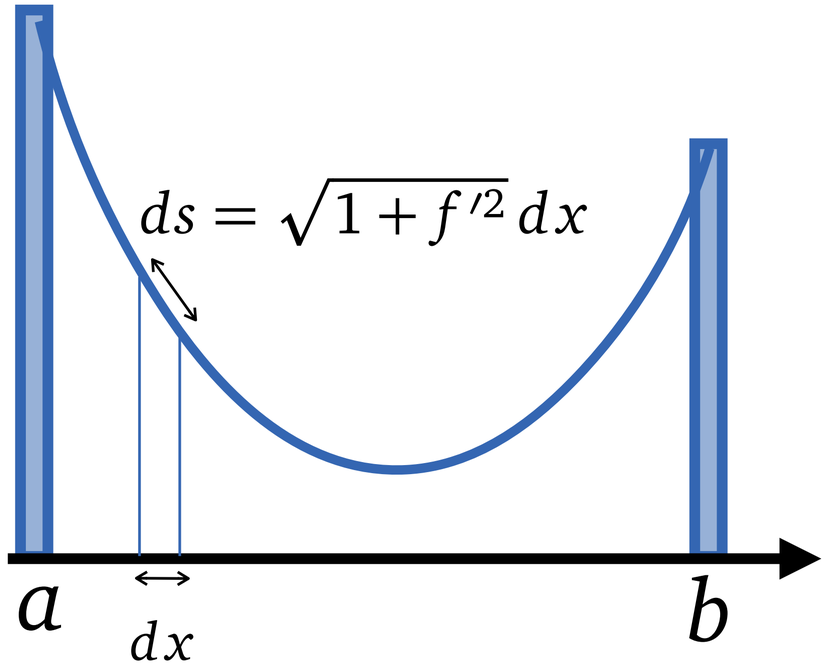
$$y = f(x)$$

- Total gravitational potential

$$\mathcal{E}(f) = \int_a^b f\sqrt{1+f'^2}\,dx$$

- Total length

$$\mathcal{L}(f) = \int_a^b \sqrt{1+f'^2}\,dx$$



- KKT condition for minimizing $\mathcal{E}$ with constraint $\mathcal{L}(f) - \ell = 0$:

There exists $\lambda \in \mathbb{R}$ such that $d\mathcal{E} + \lambda d\mathcal{L} = 0$

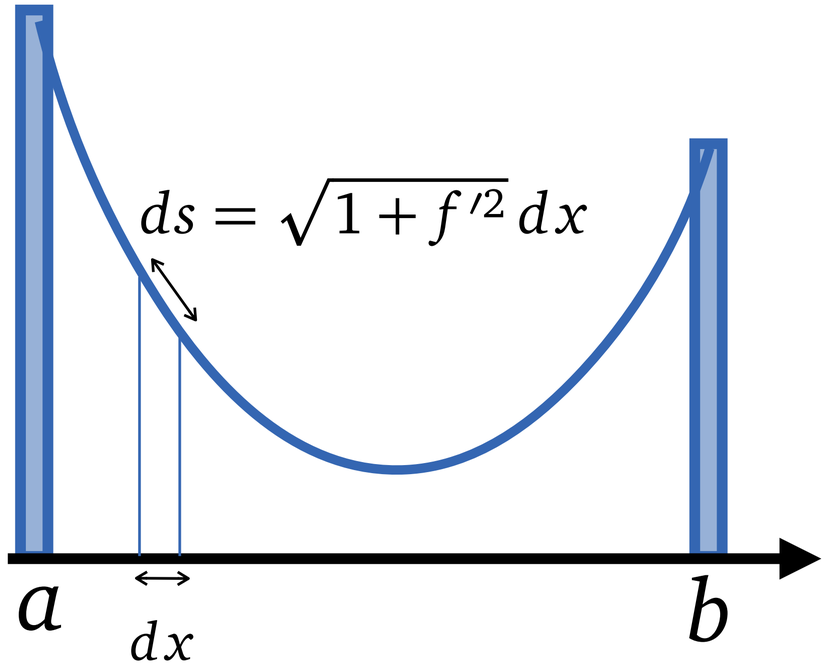
$\Leftrightarrow$ $d\widetilde{\mathcal{E}} = 0$ where $\widetilde{\mathcal{E}} = \mathcal{E} + \lambda\mathcal{L} = \int_a^b (f+\lambda)\sqrt{1+f'^2}\,dx$

Hanging chain

- Let the shape be the function graph

$$y = f(x)$$

- Minimize $\tilde{\mathcal{E}} = \int_a^b \underbrace{(f+\lambda)\sqrt{1+f'^2}}_{L(f,f')}\, dx$



- By Noether's theorem

$$\frac{\partial L}{\partial f'} f' - L = c$$

$$\Longrightarrow \quad (f+\lambda)\left(\frac{f'^2}{\sqrt{1+f'^2}} - \sqrt{1+f'^2}\right) = c$$

$$\Longrightarrow \quad f' = \pm\frac{1}{c}\sqrt{(f+\lambda)^2 - c^2}$$

first-order ODE

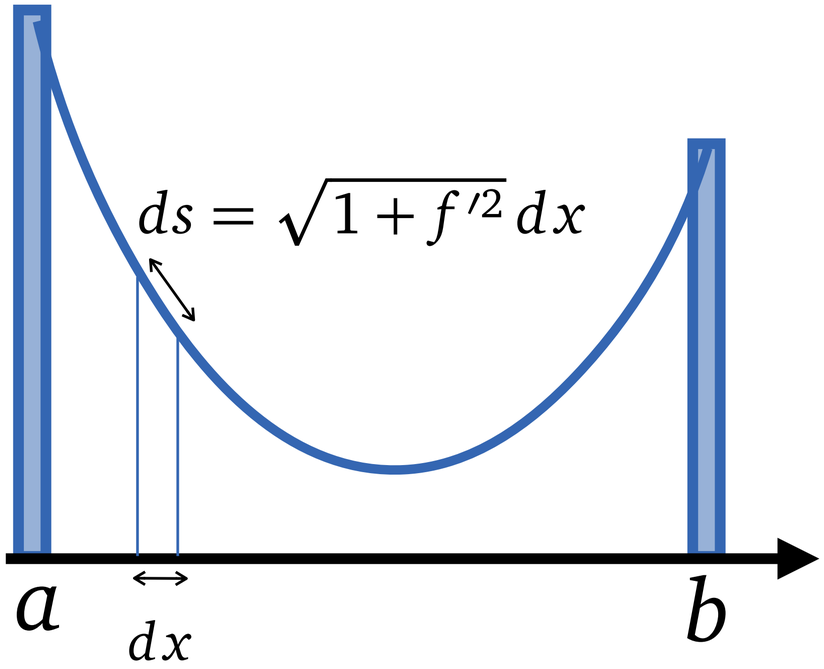
Hanging chain

$$\Longrightarrow \quad f' = \pm \frac{1}{c} \sqrt{(f+\lambda)^2 - c^2}$$

$$\Longrightarrow \quad \frac{df}{\sqrt{(f+\lambda)^2 - c^2}} = \pm \frac{dx}{c}$$

$$\Longrightarrow \quad \cosh^{-1}\left(\frac{f+\lambda}{c}\right) = \pm \frac{x}{c} + c_1$$

$$\Longrightarrow \quad \boxed{f = -\lambda + c\cosh\left(\frac{x}{c} + c_2\right)}$$

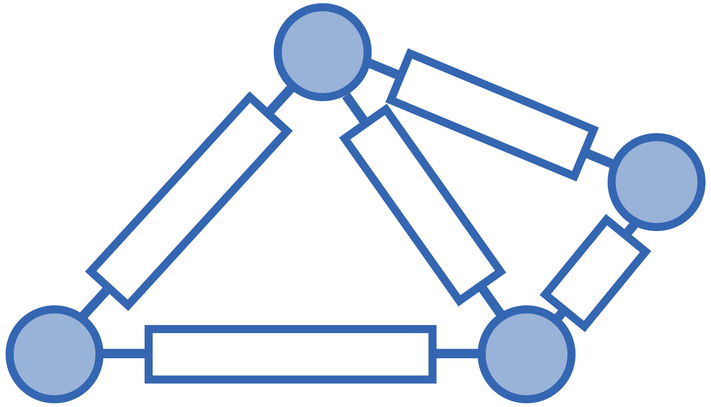


Example 4: Mass Spring System

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Mass spring system

- Consider a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$
  - Vertices are assigned with mass m_i and position $\mathbf{x}_i$
  - Edges are assigned with spring with spring constant k_e



- Total kinetic energy and potential energy

$$K = \sum_{i \in \mathcal{V}} \frac{1}{2} m_i |\dot{\mathbf{x}}_i|^2 \qquad U = \sum_{e \in \mathcal{E}} \frac{1}{2} k_e |\mathbf{x}_{\mathrm{dst}(e)} - \mathbf{x}_{\mathrm{src}(e)}|^2$$

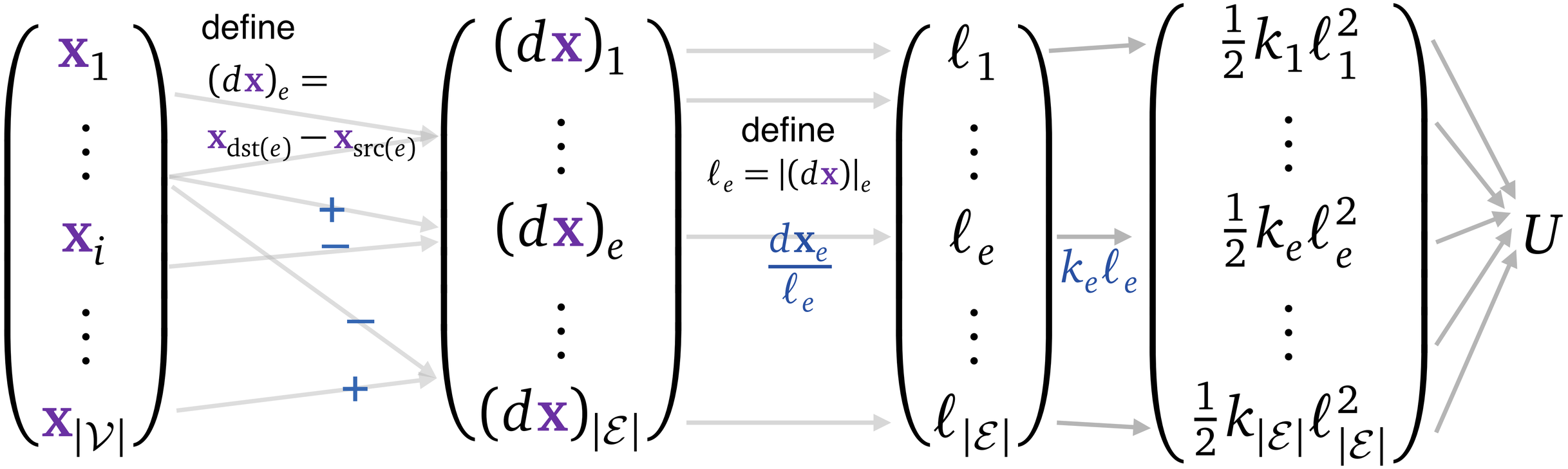
- Euler–Lagrangian equation:

$$\frac{d}{dt} \frac{\partial K}{\partial \mathbf{x}_i} = -\frac{\partial U}{\partial \mathbf{x}_i} \qquad \Longrightarrow \qquad m_i \ddot{\mathbf{x}}_i = -\frac{\partial U}{\partial \mathbf{x}_i}$$

Mass spring system

$$U = \sum_{e \in \mathcal{E}} \frac{1}{2} k_e |\mathbf{x}_{\mathrm{dst}(e)} - \mathbf{x}_{\mathrm{src}(e)}|^2$$

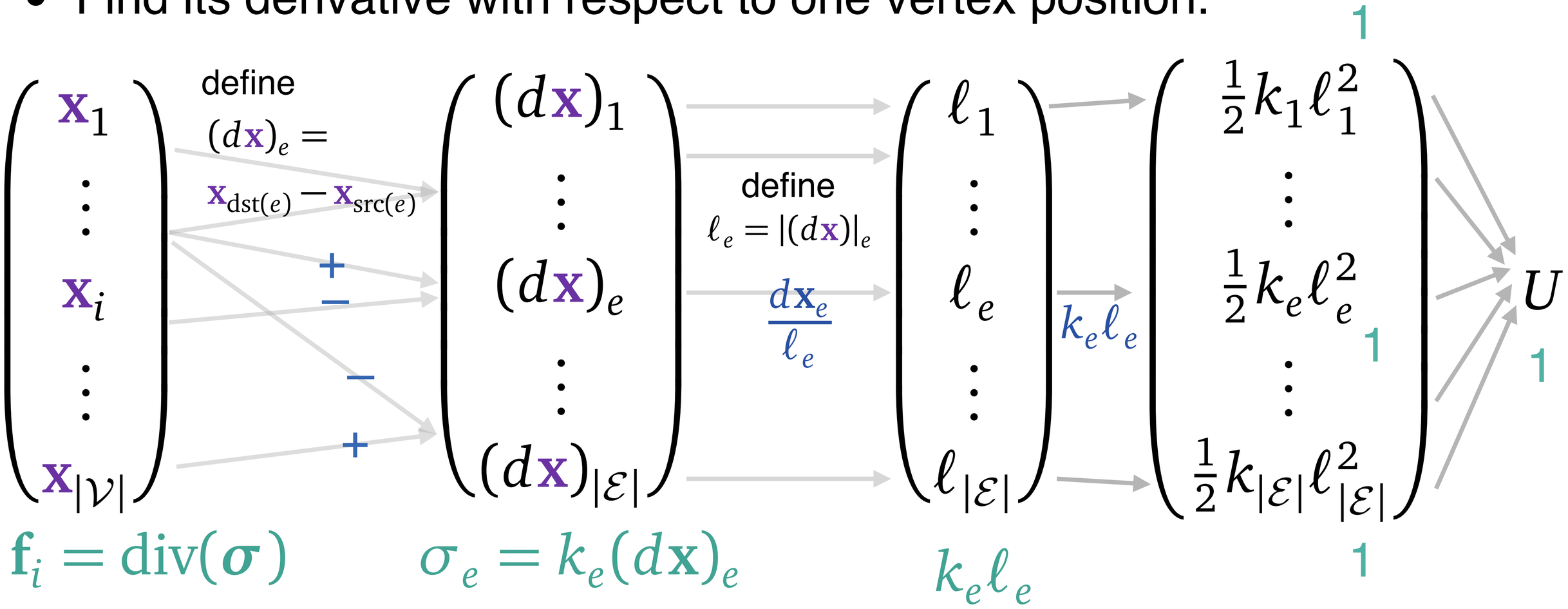
- Find its derivative with respect to one vertex position.



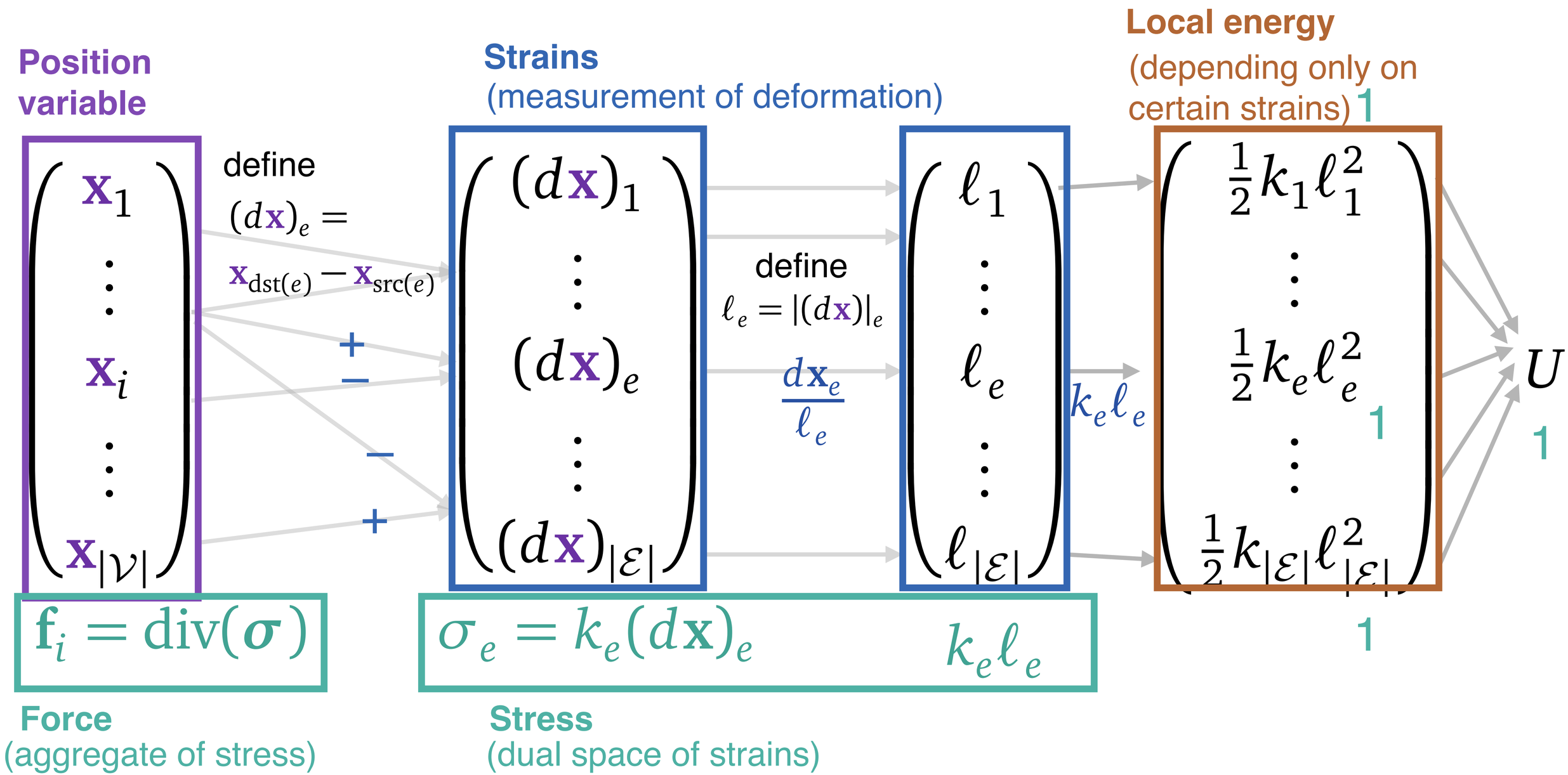
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Mass spring system



Mass spring system

$$\begin{pmatrix} m_1 & & & & \\ & \ddots & & & \\ & & m_i & & \\ & & & \ddots & \\ & & & & m_{|\mathcal{V}|} \end{pmatrix} \begin{pmatrix} \ddot{\mathbf{x}}_1 \\ \vdots \\ \ddot{\mathbf{x}}_i \\ \vdots \\ \ddot{\mathbf{x}}_{|\mathcal{V}|} \end{pmatrix} = -\mathbf{d}^\intercal \begin{pmatrix} k_1 & & & & \\ & \ddots & & & \\ & & k_e & & \\ & & & \ddots & \\ & & & & k_{|\mathcal{E}|} \end{pmatrix} \mathbf{d} \begin{pmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_i \\ \vdots \\ \mathbf{x}_{|\mathcal{V}|} \end{pmatrix}$$

graph Laplacian